SOLUTION PHASE AND COMPUTATIONAL STUDIES ON THE FORMATION, HYDROLYSIS, AND DYNAMIC EXCHANGE OF PHENYL BENZOBOROLES

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Master of Science

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by

Thusini Pavithra Hemachandra

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DEDICATION

To my family, friends, my SHSU family, and my loved ones…

ABSTRACT

Hemachandra, Thusini Pavithra. *Solution phase and computational studies on the formation, hydrolysis, and dynamic exchange of phenyl benzoboroles.* Master of Science (Chemistry), December 2021, Sam Houston State University, Huntsville, Texas.

The dynamic covalent nature of the boron-nitrogen bond of oxazaboroles and diazaboroles was investigated to gain insight into the differences in stability and the kinetics of exchange. The mechanism of hydrolysis for heteroboroles was investigated using Density Functional Theory (DFT) and Synchronous Transit-Guided Quasi-Newton (STQN) methods. This includes determining the optimized geometries, electronic and chemical properties of intermediates and transition states, and the differences in the relative stabilities of benzoxazaboroles, benzodiazaboroles, and benzodioxaboroles. In addition to the computational chemistry approach, solution-phase studies were used to explain the kinetics of exchange and the relative stabilities of heteroborole systems.

The computed Gibbs energies (ΔG) for the hydrolysis of benzoxazaborole and benzodiazaborole are -9.04 kJ/mol and -22.44 kJ/mol, respectively, which indicate that benzoxazaborole and benzodiazaborole are less stable than their hydrolysis products. The ΔG for the hydrolysis for benzodioxaborole was small (-0.14 kJ/mol), indicating that both the starting material and the products have similar stabilities.

The computational results elucidate that the hydrolysis of benzoxazaborole is preferred when the first step involves B–N bond dissociation, which had a lower energy barrier of 109.80 kJ/mol compared to that of the B-O bond dissociation (139.64 kJ/mol) during the first step. The hydrolysis of benzodiazaborole (125.66 kJ/mol) was the second-highest energy barrier out of all heteroborole hydrolysis reactions.

Further, the computational results indicate that the intermediates resulting from B-N bond dissociation during borole ring-opening were relatively lower in energy (-3.44 and 2.25 kJ/mol, respectively) compared to the intermediates resulting from B-O bond dissociation (19.41 and 10.00 kJ/mol).

In addition, similar percent conversions observed for 3-(alkyl)benzoxazaboroles and benzodioxaborole indicate that both have similar stabilities. Moreover, the equilibration between the benzodiazaborole and benzoxazaborole is very slow and a 39% conversion of benzodiazaborole was observed at equilibrium.

KEY WORDS: Density Functional Theory (DFT), Synchronous Transit-Guided Quasi-Newton (STQN) methods, Benzoxazaborole, Benzodiazaborole

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CHAPTER I

Introduction

Developments in molecular engineering and supramolecular chemistry have led to the use of non-covalent and covalent interactions to construct molecular architectures.[1] The design of molecular architectures requires careful selection of the reversible/dynamic reactions that are used in the construction of the material.[1] Molecular self-assembly, molecular recognition, host-guest chemistry, and dynamic covalent chemistry are some of the important concepts, which have grown recently with the advent of supramolecular chemistry.[1,2] Organic-based molecular architectures can be divided into three major types according to the intermolecular interaction of the building blocks, metal-organic frameworks (MOFs), supramolecular organic frameworks (SOFs), and covalent organic frameworks (COFs). In this research, we are interested in potential monomers to construct COFs.

Covalent organic frameworks

Covalent organic frameworks (COFs) are organic-based macromolecules with nanometer-sized pores.[3–6] COFs are composed of light elements (H, B, C, N, O, and S) and possess great potential in materials science due to their unique properties, such as rigid structures and strong covalent bonds,[3,4] high specific surface area, thermal stability, and low density.[7] Due to these properties, COFs have potential applications in gas storage,[8,9,10] catalysis,[11] optoelectronics,[12] chemo-sensors,[13] bio-related applications,[7,14] and nanocomposite fabrication.[10] Many COF architectures have been constructed through reversible cyclic boronate ester formation (B-O linked COFs). Yaghi and coworkers reported the pioneering work on 2D COFs, COF-1 (Figure 1) and COF-5 (Figure 2),[4] which were synthesized by

the self-condensation reaction of 1,4-benzenediboronic acid (BDBA) and through the co-condensation reaction of BDBA with 2,3,6,7,10,11-hexahydroxytriphenylene (HHTP), respectively.[4]

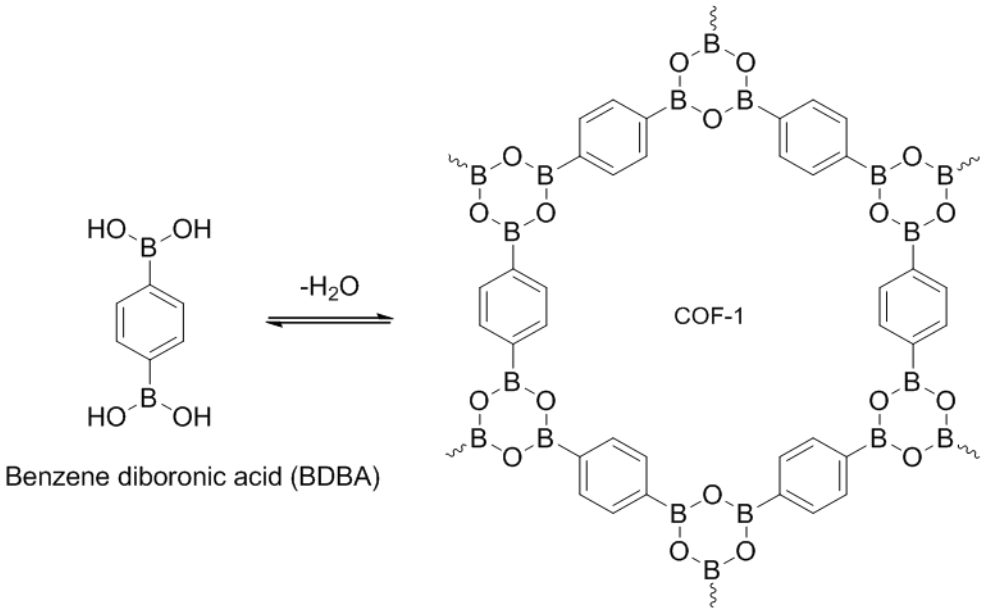


Figure 1. *Formation of COF-1*.

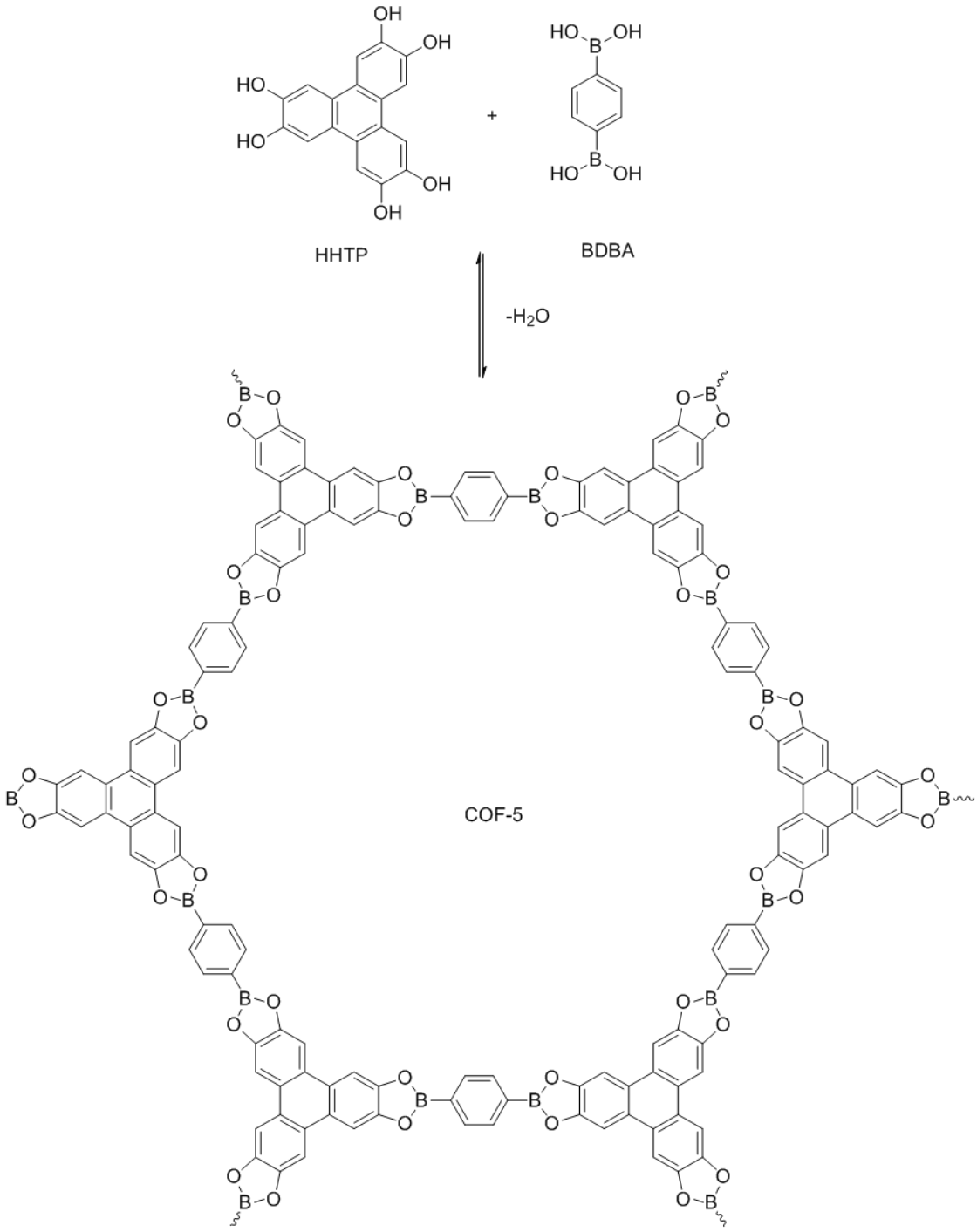


Figure 2. *Formation of COF-5.*

Dynamic covalent chemistry (DC_vC)

The synthesis of COFs has been made possible by dynamic covalent chemistry (DC_vC).[2,15,16] DC_vC is a synthetic approach that allows complex assemblies from discrete molecular building blocks to form not only COFs but a variety of molecular architectures such as macrocyclic compounds, molecular knots, polymers, and molecular capsules. High yields of the desired products are an advantage of DC_vC.[17,18] Additionally, DC_vC has been widely explored in many applications such as drug discovery, biotechnology, molecular separation, light-harvesting, gas adsorption/separation, development of self-healing systems, sensors, and actuators.[2,15,16]

In practice, DC_vC often involves a dynamic combinatorial library (DCL) of reversibly interconverting building blocks. The building blocks are spontaneously and reversibly assembled in all possible combinations, resulting in complex libraries. DCLs of different building units enable exchange processes when thermodynamics sufficiently favor the formation of one type of self-assembly over others.

Dynamic covalent reactions (DCRs) proceed through relatively low activation barriers, thus allowing both the forward and reverse reactions to take place under equilibrium conditions.[19] Because the reactions are under thermodynamic control, the distribution of the product depends only on the relative stabilities of the final products. This reversible formation and breaking of strong covalent bonds results allows for "error-checking" and "proofreading".[16] DCRs are possible with covalent bonds such as C-C, C-N, C-O, C-S, S-S, B-O, and B-N and can be categorized into two main processes; bond exchange or new bond formation.[2,16,19] Transition metal catalyzed metathesis reactions such as alkyne metathesis and olefin metathesis involve the dynamic bond exchange.

Esterification, imine formation, disulfide exchange, and boronic acid condensation are examples of DCRs involving reactions of new bond formation.[20,21]

Boron containing molecular systems

Boron-containing systems have received attention in the field of organic molecular architectures due to the superior structure-directing property of boron. This is partially due to boron's sp^2 hybridization and its ability to form compounds with trigonal planar geometry. Additionally, the empty *p* orbital on boron allows for the delocalization of π electrons, which also allows for extended π-conjugation. Recently, B-O and B-N based dynamic covalent bonds have gained interest in the field of shape-persistent molecular architectures. In this regard, our research group focuses on developing macrocycles using B-O and B-N compounds, i.e., boronate ester (dioxaborole), diazaborole, and oxazaborole based macrocycles.[22]

Boronic acids contain one alkyl or aryl group and two hydroxyl groups bonded to a central trivalent boron atom. Boronic acids are considered mild organic Lewis acids. Due to the low valency and the empty *p* orbital of the boron, boronic acids accept electron density from most Lewis bases, such as fluorides, hydroxides, amines, and carboxylates.[23,24] Moreover, boronic acids are capable of undergoing condensation reactions with compounds that possess vicinal functional groups to form boron-containing heterocycles.[25] Boronic acids and related derivatives also function as chemical building blocks for the synthesis of macromolecules and reactants in the Suzuki coupling. Additionally, the degradation of boronic acids results in the formation of non-toxic boric acid, which allows them to be considered as "green" compounds in synthetic organic chemistry.

Boronate esters (see Figure 3 for an example) are an important class of boronic acid derivatives, where the hydroxyl groups of boronic acid are replaced by alkoxy groups. Further, the significance of boron in DCRs has been shown by the inclusion of cyclic boronate esters formed by the condensation of boronic acid and a diol[24] in many designed COF architectures.[4,24]

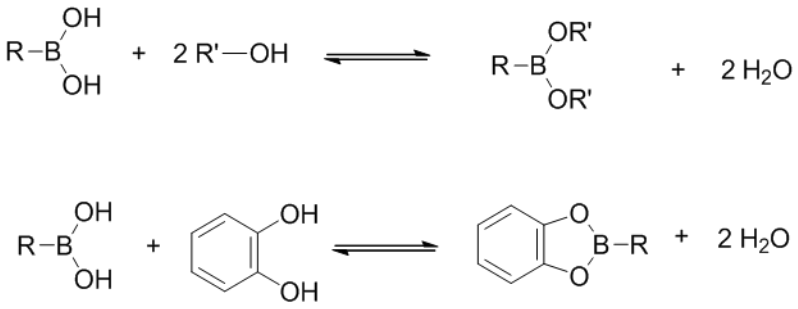


Figure 3. *Boronic acid condensation to form a) boronate esters and b) cyclic boronate esters.*

Boronate ester derivatives: phenylbenzoboroles

2-Phenylbenzoboroles are compounds that consist of two aromatic phenyl rings connected by a five-membered borole ring (see Figure 4). Depending on the heteroatoms in the borole ring, they may be classified as dioxaboroles, diazaboroles, and oxazaboroles. Dioxaboroles are formed from the condensation reaction between unsaturated 1,2-diols and boronic acids. The condensation between catechol and phenylboronic acid yields 2-phenyl-1,3,2-benzodioxaborole. To date, a considerable number of studies have been carried out to synthesize dioxaborole based macrocycles and COFs. There has been considerably less research on structurally analogous diaza or oxaza derivatives. The presence of the N atom allows for the capability of further functionalization.[24,26] For example, alkylation of the N may aid in the solubility of these compounds and may also increase the stability. The

condensation reaction between boronic acids and 2-aminophenols or benzene 1,2-diamines give rise to the formation of oxazaboroles and diazaboroles, respectively.[24]

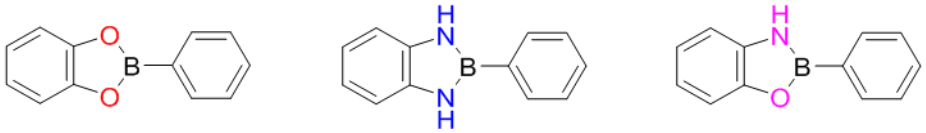


Figure 4. *Types of phenyl benzoboroles.*

The formation of 2-phenyl-1,3,2-benzodiazaborole (diazaborole) was first reported in 1958, through the reaction between *o*-phenylenediamine and dichlorophenylborane.[27] The first diazaborole-based polymer was reported in 1962 by Mulvaney and coworkers.[28] 2-phenyl-1,3,2-benzoxazaborole (benzoxazaborole) was first reported in 1958 by Dewar and coworkers. It was achieved by heating a solution of *o*-aminophenol with phenyl boron dichloride (see Figure 5).[27]

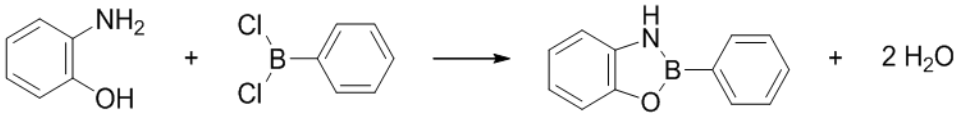


Figure 5. *Synthesis of benzoxazaborole.*

The π-conjugation of benzoboroles extends from the π-system of the phenyl ring through the five-membered borole ring, which contributes to their optoelectronic properties. Computational investigations of benzoxazaborole and benzodiazaborole have previously been conducted to examine these electronic properties of the conjugated systems.[29,30] The vacant *p* orbital of the boron allows for extended π-conjugation, which decreases the HOMO-LUMO gap,[31] causing blue luminescence when it is irradiated with UV light.[32] Due to these properties, benzoboroles have potential applications in wide areas such as linear and nonlinear optics,[33] organic semiconductors,[34] luminescent polymers, and probes for anions,[32] emissive materials,[35] as well as photoluminescent materials.[36,37] The

investigation of novel boron-nitrogen-linked macrocycle systems is further motivated by such applications.

Summary of previous work

The dynamic covalent nature of B-N derivatized boronate esters has been studied by ^{1}H NMR spectroscopy and computationally by exchanging various heteroboroles with either 1,2- and 1,3-diols, 1,2-diamines, or 2-aminoalcohols.[29,38] The equilibrium constant (K_{eq}) and Gibbs free energy values of the exchange reactions were calculated. Self-assembly of 3-(alkyl)benzoxazaborole was studied by former group member Chathurika Rathnayaka. The results showed that the stability of 3-(alkyl)benzoxazaboroles is not dependent on the length of the alkyl chain. Similarly, another study was carried out to find the relative stability of 3-(alkyl)benzoxazaborole and benzodioxaborole (see Figure 6).[29]

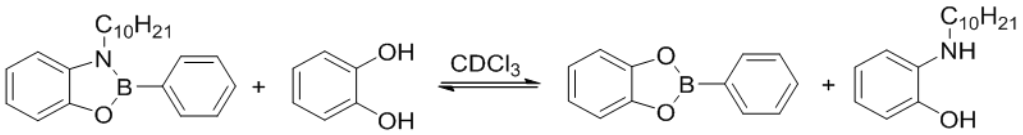


Figure 6. *The dynamic reaction of 3-(decyl)benzoxazaborole with catechol.*

The average experimental K_{eq} and ΔG for the above reaction were found to be 1.28±0.41 and -0.61±0.92 kJ/mol, respectively. The computationally calculated ΔG for the same reaction was -8.00 kJ/mol. The experimental and computational results revealed that 3-(alkyl)benzoxazaborole and benzodioxaborole have similar stability.[29]

Former group member Sobiya George studied and demonstrated that diazaboroles also exhibit dynamic covalent behavior by analyzing the relative stabilities of 3-(alkyl)benzoxazaborole and benzodioxaborole using NMR spectroscopy.[30,38] The ^{1}H NMR results revealed that the reaction between 2-(decylamino)phenol and diazaborole (Figure 7) is slow, which took over a week to establish equilibrium. This was comparatively much

slower than that of the dioxaborole equilibration, and the reaction eventually reached 90% conversion (K_{eq} = 81).[38]

Figure 7. *The reaction of diazaborole and 2-(decylamino)phenol.*

To further support the above observations 2-(decylamino)phenol, catechol, benzene-1,2-diamine, and phenylboronic acid were mixed in an equal molar ratio (Figure 8). After equilibrating, the ratio between dioxaborole : oxazaborole : diazaborole was found to be 4.5:4.5:1. This result supported the previous finding that dioxaborole and alkyl oxazaborole have similar stabilities and both are more stable than diazaborole.[38]

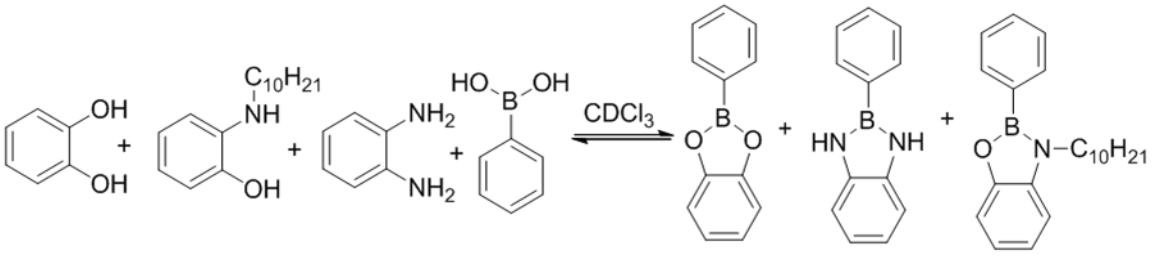


Figure 8. *A dynamic covalent library: the formation of benzodioxaborole, benzodiazaborole, and 3-(decyl)benzoxazaborole.*

Aims of this research

The previously reported observations led us to explore the reasons for differences in the thermodynamic stability and rates of formation and exchange of heteroboroles.[29,38] A combined spectroscopic and computational investigation of the self-assembly of benzoboroles was performed to discover the influence of different organic donors (catechol, benzene-1,2-diamine, and 2-(ethylamino)phenol) during exchange reactions (see i-iii Figure 9). The Gibbs free energy and equilibrium constants of these heteroborole

exchange reactions were determined both experimentally, using NMR spectroscopy, and computationally.

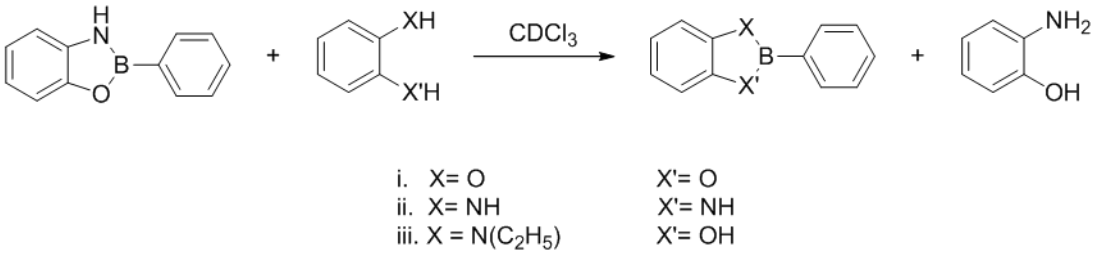


Figure 9. *Dynamic covalent reactions of heteroboroles.*

Further, we initiated the present study to evaluate the potential intermediate structures that might exist during the formation of heteroboroles with the expectation of elucidating insight into the mechanism of their formation. Most recently, a similar computational study was conducted with to determine the hydrolytic stability of boronate ester linked COF-5 unit TDPBA, 4-(2,3,6,7-tetrahydroxytriphenyleno[2,3-*d*][1,3,2]dioxaborol-11-yl)phenylboronic acid. The associated mechanism of hydrolysis is investigated based on the dissociation reaction of the COF-5 unit via reaction pathway analysis using density functional theory calculations. In addition, the impact of the presence and number of water molecules, and the environment of the neighboring COF-5 fragments upon hydrolysis was also examined.[39] In our work, the hydrolysis (and the reverse reaction, formation) of simple heteroboroles was studied computationally (Figure 10). This included studying the potential intermediates, modeling the corresponding transition states, analyzing the most reasonable pathways, and the rate-determining step.

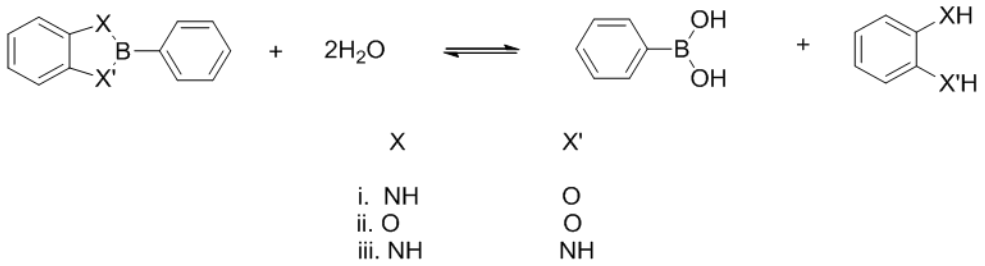


Figure 10. *Hydrolysis of heteroboroles.*

Experimental and computational results were then combined to rationalize the reasons for differences in heteroborole exchange. Computational chemistry was used to support the experimental results of the self-assembly of phenyl benzoboroles. Finally, the combined computational and experimental results provided insight into the mechanism of formation/hydrolysis, as well as optimized geometries, electronic and chemical properties of intermediates, and transition states. Therefore, this research will help to clarify the potential use of B-N-based heteroboroles in molecular architecture.

CHAPTER II

Exchange Reactions of Oxazaborole, Dioxaborole, and Diazaborole

Introduction

Dynamic covalent reversibility is an important feature during the synthesis of boron-nitrogen-based molecular architectures. Former group members have studied the dynamic nature of 3-(alkyl)benzoxazaboroles and benzodiazaborole, and their relative stabilities were compared with benzodioxaborole. These dynamic reactions were studied using ^{1}H NMR spectroscopy and computationally, and the equilibrium constant and Gibbs free energy values of the exchange reactions were calculated. Despite these efforts, the dynamic covalent nature of simple benzoxazaborole **2.1** has not been thoroughly investigated.

Objectives

The purpose of this project was to analyze the stability and the dynamic covalent nature of 2-phenyl-2,3-dihydro-1H-1,3,2-benzoxazaborole (**2.1**). The solution phase exchange reactions of benzoxazaborole **2.1** with benzene-1,2-diol (catechol) and benzene-1,2-diamine were investigated to determine the equilibrium constants and Gibbs free energy values of these exchange reactions.

Solution study on the benzoborole exchange

To investigate the relative stabilities of benzoxazaborole **2.1** and benzodioxaborole **2.3**, direct mixing experiments were carried out. Benzoxazaborole **2.1** and catechol **2.2** were mixed in a 1:1 ratio in $CDCl_3$ (Figure 11). Upon mixing, a white precipitate formed. The mixture reached apparent steady-state conditions within 2h, and there was no visible change in the ^{1}H NMR spectrum over the next 24 hours.

Figure 11. *The reaction of benzoxazaborole **2.1** and catechol (**2.2**).*

In the ^{1}H NMR spectrum of the reaction mixture, signals corresponding to both starting materials and products were observed (Figure 12). There was a clear decrease of the signals at 7.3 and 7.1 ppm, which correspond to the protons of the fused "benzo" ring of **2.1**, and only a slight appearance of signals near 6.7 that correspond to the aromatic protons of **2.4**, which supports the notion that the 2-aminophenol was the precipitate. The ratio of **2.1** to **2.3** was determined by integrating the protons ortho to the boron atom (H_a of **2.1** and (H_b of **2.3**). When comparing the results for three separate reaction runs, the percent conversion was calculated to be 91 ± 2%, which was much greater than the previous studies involving 3-(alkyl)benzoxazaboroles that showed a conversion of 50%.[29] This observation indicates that the precipitation of 2-aminophenol greatly influences the equilibrium and causes an increase in the formation of benzodioxaborole **2.3**, as would be expected by Le Chatelier's Principle.

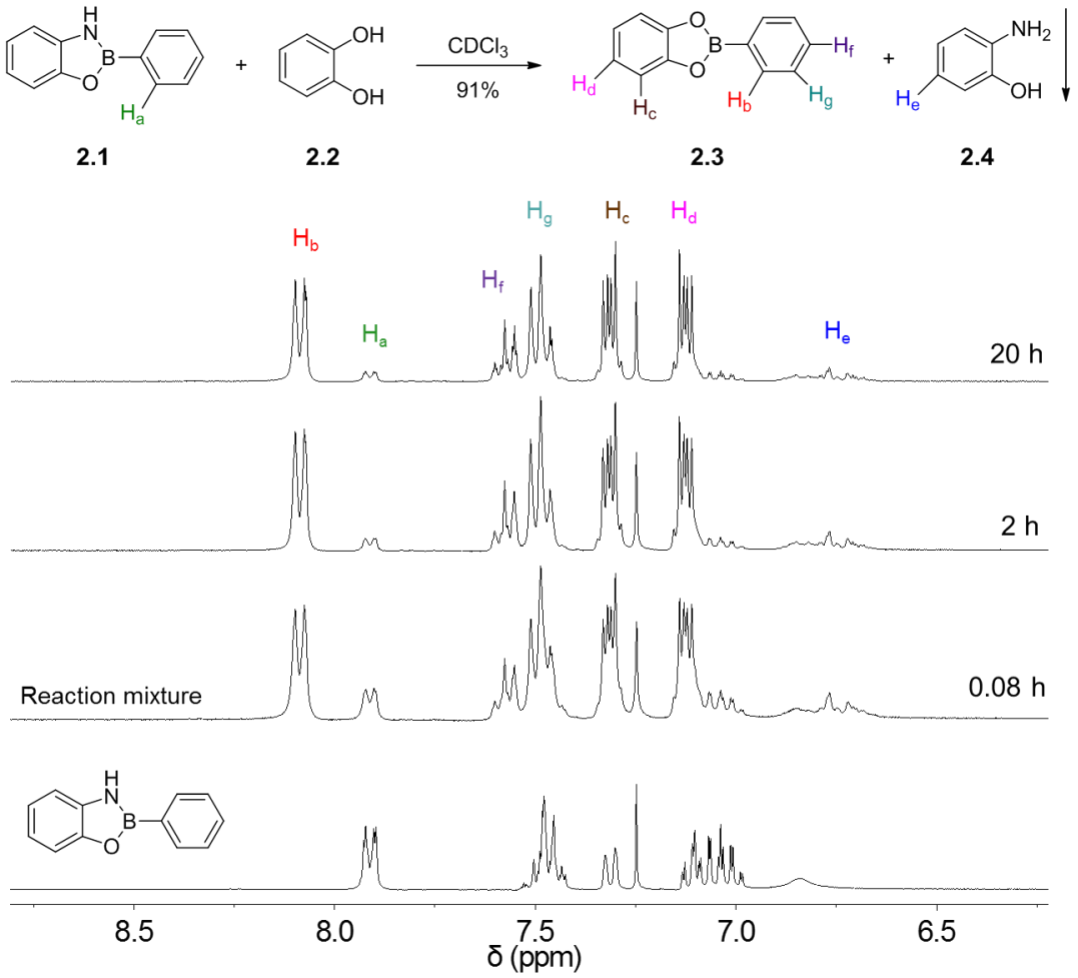


Figure 12. *Stacked [1]H NMR spectra of the reaction of benzoxazaborole **2.1** and catechol (**2.2**) in $CDCl_3$.*

The following reaction (Figure 13) was carried out to analyze the relative stabilities of benzoxazaborole **2.1** and benzodiazaborole **2.6**. In an NMR tube, a 1:1 ratio of benzoxazaborole **2.1** and benzene-1,2-diamine (**2.5**) were mixed in $CDCl_3$ and the reaction mixture was monitored using ^{1}H NMR.

Figure 13. *The reaction of benzoxazaborole **2.1** and benzene-1,2-diamine (**2.5**).*

In the ^{1}H NMR spectrum of the reaction mixture, signals corresponding to both starting materials and products were observed (Figure 14). In this case, the reaction was much slower than that of the reaction involving catechol (Figure 11). Over time, a white precipitate, presumed to be 2-aminophenol, formed indicating that the reaction was likely proceeding in the forward direction. The relative amounts of benzoxazaborole and benzodiazaborole were determined by integrating the protons ortho to the boron atom in benzoxazaborole **2.1** (H_a) and benzodiazaborole **2.6** (H_b).

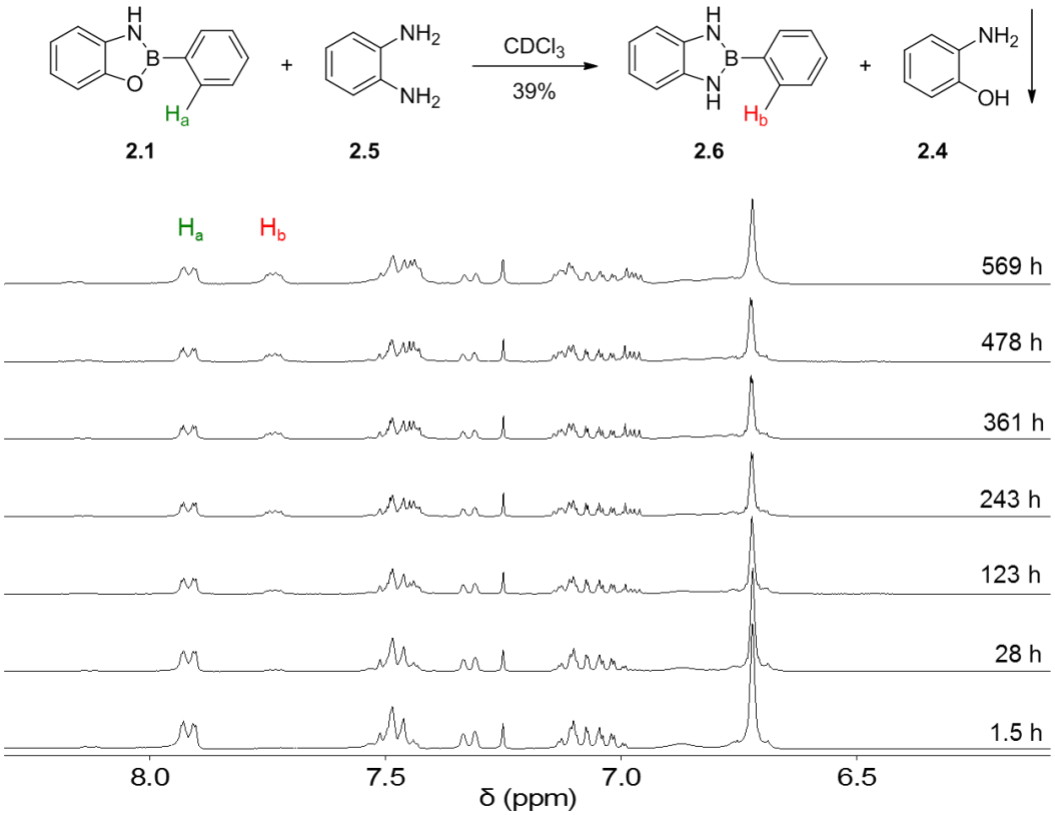


Figure 14. *Stacked ^{1}H NMR spectra of the reaction of benzoxazaborole **2.1** and benzene-1,2-diamine (**2.5**) in $CDCl_3$.*

By comparing the integral values of benzoxazaborole **2.1** and benzodiazaborole **2.6**, the percent conversion was calculated and then plotted versus time (Figure 15). Apparent equilibrium took more than two weeks, and a 39% conversion to benzodiazaborole **2.6** was observed. The percent conversion was much greater than the previous studies involving 3-(alkyl)benzoxazaboroles that showed a conversion of 10% for the analogous reaction.[38] This observation indicates that the precipitation of 2-aminophenol greatly affects the equilibrium and causes an increase in the formation of **2.6**.

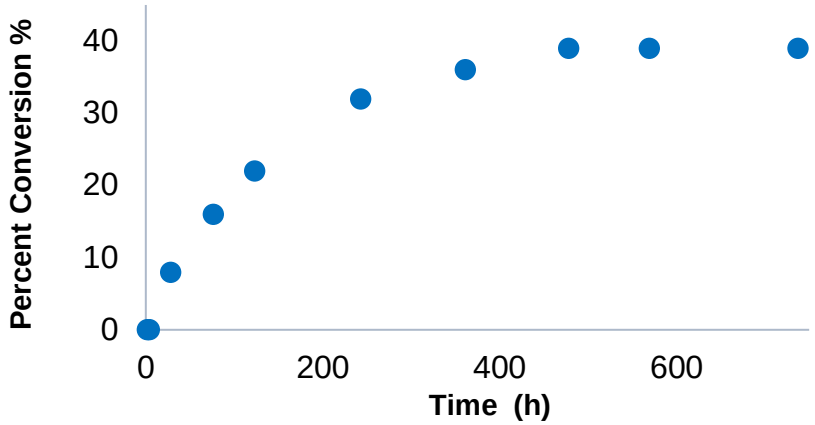


Figure 15. *The percent conversion to benzodiazaborole **2.6** over time.*

To investigate the relative stability of benzoxazaborole compared to 3-(alkyl)benzoxazaborole, direct mixing experiments were carried out. Benzoxazaborole **2.1** and 2-(ethylamino)phenol (**2.7**) were mixed in a 1:1 ratio in $CDCl_3$ (Figure 16). When mixing benzoxazaborole **2.1** and 2-(ethylamino)phenol (**2.7**) a white precipitate presumed to be 2-aminophenol formed rapidly similar to the reaction between benzoxazaborole **2.1** and catechol (**2.2**) described above.

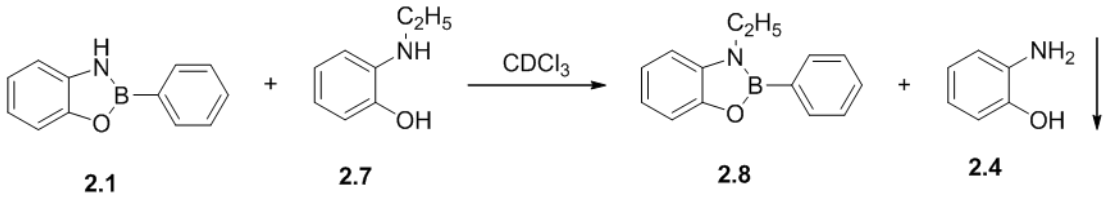


Figure 16. *The reaction of benzoxazaborole **2.1** and 2-(ethylamino)phenol (**2.7**).*

Apparent steady-state conditions were reached within five minutes, and there was no observable change in the ^{1}H NMR spectrum over the following 24 hours. In the ^{1}H NMR spectrum of the reaction mixture, signals corresponding to both of the starting materials and products were observed (Figure 17). The signals for the protons ortho to the boron atom were indistinguishable due to their similar chemical environments. Therefore, the ratio of starting materials and products was determined by integrating the methylene

protons of 2-(ethylamino)phenol (**2.7**) (H_a), and 3-(ethyl)benzoxazaborole **2.8** (H_b). When comparing the results for three separate reaction runs, the percent conversion was calculated to be 92 ± 1% of 2-(ethylamino)phenol (**2.7**) (H_a) (and thereby benzoxazaborole **2.1** was converted to 3-(ethyl)benzoxazaborole **2.8** (H_b), which was much greater than the previous studies involving 3-(alkyl)benzoxazaboroles that showed a conversion of 50%.[29] This observation indicates that the precipitation of 2-aminophenol greatly influences the equilibrium and causes an increase in the formation of 3-(ethyl)benzodioxaborole **2.8**.

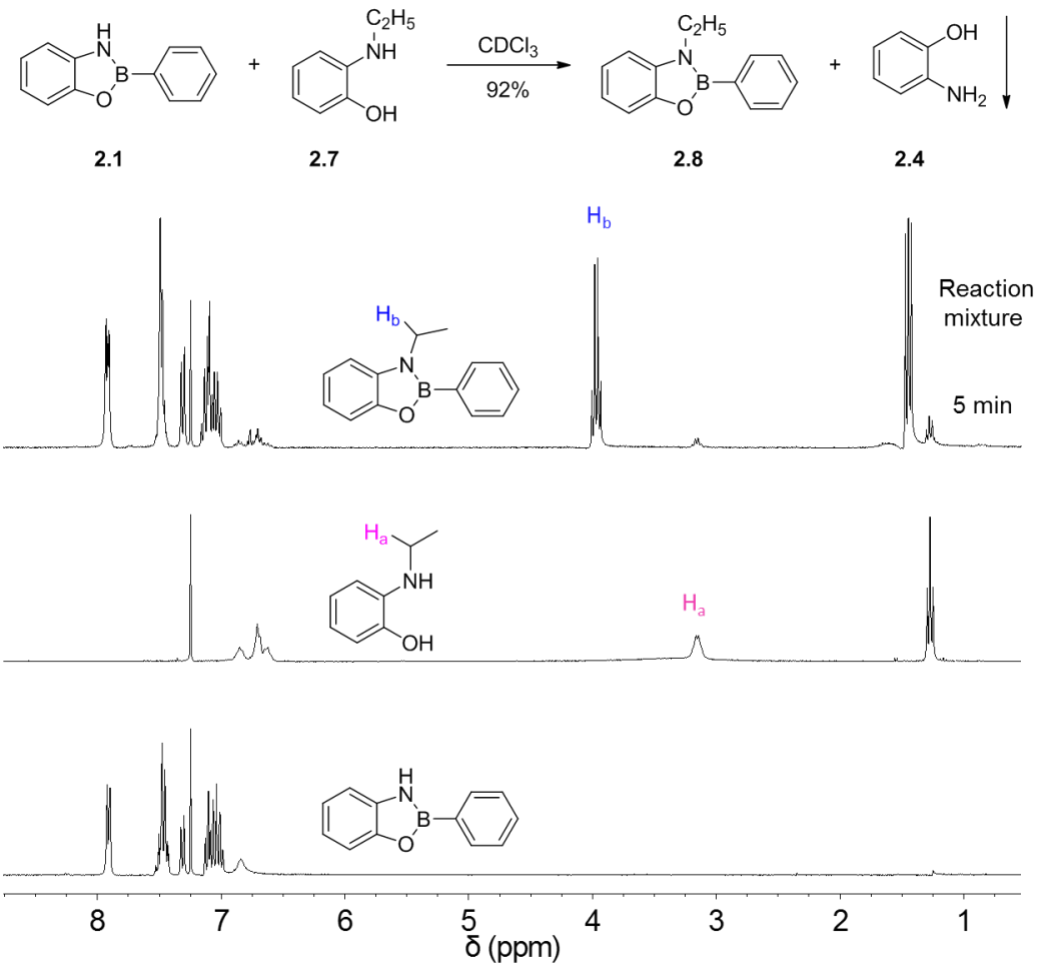


Figure 17. *Stacked [1]H NMR spectra of the reaction of benzoxazaborole **2.1** and 3-(ethylamino)phenol (**2.7**) in $CDCl_3$, along with spectra of the individual starting materials, benzoxazaborole **2.1** and 3-(ethylamino)phenol (**2.7**).*

In previous studies, we found that a 1:1 mixture of 3-(alkyl)benzoxazaborole and catechol results in a 1:1 ratio (50% conversion) of benzodioxaborole and 3-(alkyl)benzoxazaborole at equilibrium.[29] In that case, all components, including the 2-(alkylamino)phenol, remained in solution and did not affect the chemical equilibrium. Because the reactions between the non(alkyl)benzoxazaborole **2.1** and catechol (**2.2**) or 2-(ethylamino)phenol (**2.7**) had similar conversions, 91 ± 2%, and 92 ± 1%, respectively, the

previous findings[29,38] that the two species 3-(alkyl)benzoxazaboroles and benzodioxaborole) have similar stabilities is supported (see Table 1 for a summary).

Table 1. *Percent conversion values for the exchange reactions of non(alkyl)benzoxazaborole **2.1**.*

Reaction	Percent conversion (%)
2.1 + 2.2	91 ± 2
2.1 + 2.5	39
2.1 + 2.7	92 ± 1

Computational study on benzoborole exchange

The exchange reactions discussed above-involving non(alkyl)benzoxazaborole result in the precipitation of 2-aminophenol, which affects the chemical equilibrium, and drives the reaction in the forward direction (see Figure 18 for a summary).

Reaction	X	X'	Reactant		Product	
1	O	O	catechol	**2.2**	benzodioxaborole	**2.3**
2	NH	NH	benzene-1,2-diamine	**2.5**	benzodiazaborole	**2.6**
3	$N(C_2H_5)$	O	2-(ethylamino)phenol	**2.7**	3-(ethyl)benzoxazaborole	**2.8**

Figure 18. *Reactions of benzoxazaborole **2.1**.*

Due to the poor solubility of 2-aminophenol in chloroform, studying the exchange reactions of benzoxazaborole **2.1** using NMR spectroscopy in this solvent is limited. To address this limitation a computational study was carried out to determine the equilibrium constant (K_{eq}) and the Gibbs free energy (ΔG°) of the exchange reactions. The zero-point

corrected Gibbs free energies of exchange ($\Delta G^{\circ}_{exchange}$) of benzoboroles at room temperature (298 K) and pressure at 1.00 atm were calculated using the equation: $\Delta G^{\circ}_{exchange} = G^{\circ}_{products} - G^{\circ}_{reactants}$.

In 2016, Northrop and Goldberg reported the Gibbs free energy values of formation ($\Delta G_{formation}$) for tertiary butyl substituted diazaborole derivatives using the four levels of theories (Density Functional Theory /B3LYP/6-311+G(d,p), M06-2X/6-31+G(d,p), CBS-QB3, and MP2/aug-cc-PVDZ) in chloroform (ε=4.7113) using polarizable continuum model (PCM) and compared them with experimental results.[40] Former members of our research group performed thermodynamic calculations on several diazaborole and (alkyl)oxazaborole exchange reactions in different solvent models and the gas phase, respectively using Density Functional Theory (DFT) with the B3LYP/6-311++G(d,p) functional and basis set.[29,30] The ΔG for the formation of diazaborole analogues is favorable in THF, acetonitrile, methanol, 1,4-dioxane, and 1-butanol compared to the gas phase, whereas the reverse was observed in chloroform and DMSO.[30] The previous findings on exchange reactions involving 3-(alkyl)benzoxazaborole indicate that the computed ΔG was small suggesting that is no significant difference in energy between 3-(alkyl)benzoxazaborole and benzodioxaborole for exchange reactions.[29]

In the present study, we are interested in the computational calculations on the exchange reactions of non(alkyl)benzoxazaboroles in the chloroform solvent model and gas phase. The density functional theory (DFT) method, and the model chemistry as B3LYP functional with either 6-311+G or 6-311++G(d,p) basis sets were used to perform all optimization and frequency calculations, the default SCRF (self-consistent reaction field) method was used as the solvent model. The numbers in the basis set (6-311G)

indicate that the six Gaussian functions are summed to describe the inner shell orbital (core electrons) and three Slater type orbitals (triple zeta), comprised of 3, 1, and 1 Gaussian functions, respectively, are used to describe the valence electrons of the molecule. Additional functions are added to describe the polarization of the electron density of the atoms in a molecule. Specifically, *d*-orbitals for the heavy atoms in and *p* for the orbitals for the hydrogen were made available to accommodate polarization to reach more accurate results. Further, a diffuse function (+) was employed to capture the total electron distribution of atoms due to the presence of lone pair electrons on the heteroatoms of heteroboroles.

Previously, as described in Chapter 1, the dynamic nature of 3-(alkyl)benzoxazaboroles and benzodiazaborole was studied, and the experimental results were supported by calculations using the diffuse functions on both heavy atoms and hydrogen (6-311++G(d,p)) in the gas phase (see Figure 6).[29] Therefore, to compare the current results involving reactions of non(alkyl)benzoxazaborole **2.1** with previous results we include results from both basis sets, 6-311+G(d,p) and 6-311++G(d,p).

The Gibbs free energy (ΔG) of the exchange reactions involving non(alkyl)benzoxazaborole **2.1** are shown in Table 2. On average, the exchange reaction involving benzoxazaborole **2.1** to give benzodioxaborole **2.3** (reaction 1), has favorable ΔG values and the reaction of benzoxazaborole **2.1** to give 3-(ethyl)benzoxazaborole **2.8** (reaction 3) has a relatively small ΔG value except for reaction in chloroform using 6-311++G(d,p) basis set, while the exchange of benzoxazaborole **2.1** to give benzodiazaborole **2.6** (reaction 2) has an unfavorable/endergonic ΔG under all conditions.

The Δ*G* values for all three reactions using either method are more favorable in the gas phase compared to the chloroform solvent model.

Table 2. *Gibbs free energy for the exchange reactions of non(alkyl)benzoxazaborole **2.1** using DFT/B3LYP with the 6-311+G(d,p) and 6-311++G(d,p) basis sets.*

Reaction	Δ*G* (kJ/mol)			
	6-311+G(d,p)		6-311++G(d,p)	
	$CHCl_3$	gas phase	$CHCl_3$	gas phase
2.1 + 2.2	-1.51	-8.55	-1.67	-9.04
2.1 + 2.5	9.89	7.97	10.20	8.04
2.1 + 2.7	2.12	-0.27	7.46	0.10

Upon examining the computed Δ*G* results and experimental observations obtained for reactions 1-3, it is clear that computational calculations support the experimental NMR results, where reactions 1 and 3 were relatively more favorable, having percent conversions of 91 ± 2% and 92 ± 1%, respectively, and reaction 2 was relatively less favorable having 39% conversion.

To compare the current results with previous results, the Δ*G* for reaction 1 was studied. The computed Δ*G* values for non(alkyl)oxazaborole **2.1** and catechol (**2.2**) in the gas phase using the 6-311G+(d,p) and 6-311++G(d,p) basis sets are -8.55 kJ/mol and -9.04 kJ/mol, respectively. This small energy difference (ΔΔ*G* = 0.49 kJ/mol) for the two basis sets, indicates that the effect of the diffuse function is minimal. Previously, the Δ*G* values for 3-(alkyl)benzoxazaboroles and catechol (**2.2**) were studied using the 6-311++G(d,p) method in the gas phase, and it was found to be -8.00 kJ/mol.[29] (see Figure 6). Accordingly, the previously computed Δ*G* is in line with the results (Δ*G*) obtained for reaction 1 in the

gas phase for both basis sets. However, a comparison of the current and previous Δ*G* values obtained for reaction 3 indicates that there is no significant difference between the stability of non(alkyl)benzoxazaborole (**2.1**) and (alkyl)benzoxazaborole (**2.8**) except for the computed Δ*G* value using the basis set 6-311++G(d,p) in CHCl3, and which appears to be an outlier.

Conclusion

The exchange reactions involving non(alkyl)benzoxazaborole **2.1** with benzodioxaborole **2.3**, and alkyl oxazaborole **2.8** are rapid and apparent equilibrium was achieved soon after mixing the reactants. The equilibration between the benzodiazaborole **2.6** and benzoxazaborole **2.1** is very slow and apparent equilibrium was reached after approximately two weeks.

The reaction between benzoxazaborole **2.1** and catechol (**2.2**) resulted in a 91 ± 2% conversion to benzodioxaborole, similarly, the reaction between benzoxazaborole **2.1** and 2-(ethylamino)phenol (**2.7**) resulted in a 92 ± 1% conversion to 3-(ethyl)benzoxazaborole **2.8**. The similar percent conversions also support the previous results that the two species (3-(alkyl)benzoxazaboroles and benzodioxaborole) have similar stabilities.[29] The reaction between benzoxazaborole **2.1** and benzene-1,2-diamine (**2.5**) had a much greater percent conversion (39%) compared to the previous studies involving the analogous reaction 3-(alkyl)benzoxazaboroles.[38] These observations indicate that the precipitation of 2-aminophenol greatly influences the equilibrium and causes an increase in the formation of products in all three reactions.

Computed thermodynamic data were also used to support the previous observations and the stability of benzodiazaborole **2.6** is lower than that of the

non(alkyl)benzoxazaborole **2.1**. Upon comparing the Δ*G* values using the two basis sets presented in Table 2, the computational results at the 6-311+G(d,p) level are the most consistent with the experimental data.

Moreover, the exchange reaction involving 3-(alkyl)benzoxazaborole and benzodioxaborole (Figure 6) suggest that the relative stabilities of 3-(alkyl)benzoxazaborole and benzodioxaborole are higher than that of the stability of the non(alkyl)oxazaborole **2.1**. In addition, according to reaction 2 in Table 2 and previous studies (Figure 7)[38] the stability of benzodiazaborole is less stable than that of the 3-(alkyl)benzoxazaborole.

Experimental section

Chemicals and reagents. Benzoxazaborole **2.1** was synthesized similar to a previous method.[29] 2-(ethyl)aminophenol (**2.7**) was synthesized by former group member Chathurika Rathnayaka.[29] Catechol (**2.2**) and benzene-1,2-diamine (**2.5**) were purchased from Alfa Aesar and used without further purification. The $CDCl_3$ was purchased from Magnisolv and stored over 3 Å molecular sieves.

NMR spectroscopy. The ^{1}H and ^{13}C NMR spectra were collected on a JEOL Eclipse 300+ spectrometer. Chemical shifts are reported in δ (ppm) relative to the residual solvent signal for ^{1}H ($CHCl_3$: 7.26) and the splitting patterns are designated as s (singlet), d (doublet), t (triplet), q (quartet), and m (multiplet).

Computational calculations. All computational calculations were performed with the Gaussian G09W suite of programs. Originally, the molecular structures were built within the GaussView 5.0.9 interface, and the geometric optimization was run using the density functional theory (DFT) and B3LYP functional with either the 6-311+G(d,p) or 6-

311++G(d,p) basis set in both the gas phase and chloroform using the default SCRF (self-consistent reaction field) solvent model. The optimized geometries were then subjected to frequency calculations at the same level of theory.[41,42]

Synthesis of 2-phenyl-1,3,2-benzoxazaborole (benzoxazaborole 2.1).

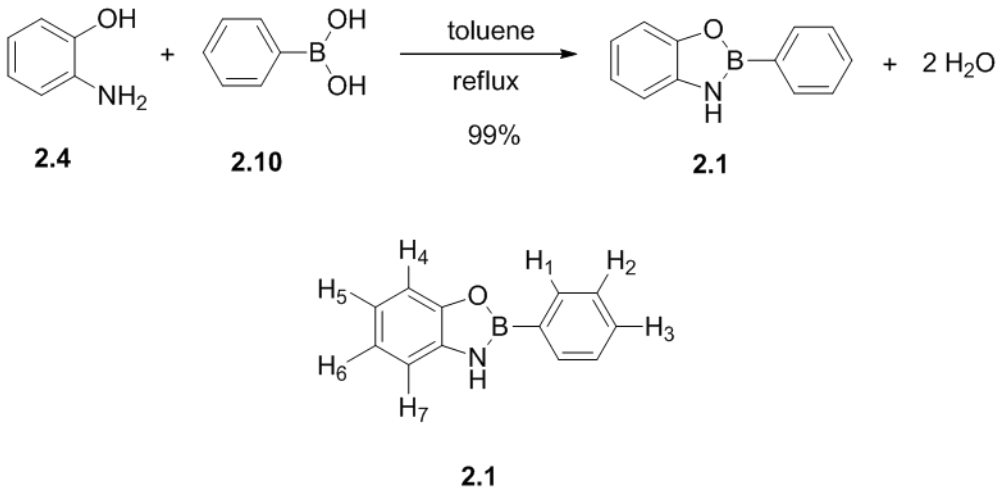


Figure 19. *Synthesis of benzoxazaborole **2.1** using 2-aminophenol (**2.4**) and phenylboronic acid (**2.10**).*

Using a method similar to previous work,[29] a 50 ml round bottom flask was loaded with phenylboronic acid (244 mg, 2.0 mmol, 1 equiv) and 2-aminophenol (218 mg, 2.0 mmol, 1 equiv), and toluene (30 ml). The reaction mixture was refluxed connected to a Dean-Stark apparatus for 8h. Then, the solvent was removed under reduced pressure using (27 in Hg) a rotary evaporator at 45 °C to give an amorphous white solid (383 mg, 97% yield). ^{1}H NMR data (300 MHz, $CDCl_3$,): δ = 7.92 (d, 2H, ArH_1), 7.54-7.42 (m, 3H, ArH_2, H_3), 7.32 (d, 1H, ArH_7), 7.16-6.98 (m, 3H, $ArH_{4,5,6}$), 6.86-6.66 (m, 4H, ArH).

Reaction of 2-phenyl-2,3-dihydro-1H-1,3,2-benzoxazaborole (**2.1**) **and catechol** (**2.2**). Benzoxazaborole **2.1** (9.8 mg, 0.05 mmol, 1 equiv) and catechol (**2.2**) (5.5 mg, 0.05 mmol, 1 equiv), and $CDCl_3$ (0.7 ml) were combined in NMR tube and the reaction progress was

monitored using ^{1}H NMR spectroscopy. This was repeated a total of three times at the same concentration. There was no difference in the spectra collected at 2h and 24h (see Figure 12). Partial ^{1}H NMR (300 MHz, $CDCl_3$,) δ 8.10 (d, ArH (**2.3**)), 7.92 (d, ArH (**2.1**)).

$$\text{Percent conversion} = \frac{\text{Integration of (2.3) at } \delta\ 8.10}{\text{Integration of (2.1) at } \delta\ 7.92 + \text{(2.3) at } \delta\ 8.10 + \text{boron-containing intermediates at } \delta\ 8.35\text{-}7.75} * 100\%$$

Table 3. *^{1}H NMR signals and integrations used to determine the percent conversion of benzodioxaborole **2.3**.*

Trial	Reactant (**2.1**) H_a δ 7.92 (d)	Product (**2.3**) H_b δ 8.10 (d)	Boron containing intermediates δ (8.35)+(7.80)+(7.75)	Percent conversion (%)
i	0.0806	1.00	0.0175	91.0
ii	0.1100	1.00	0.0116	89.1
iii	0.0611	1.00	0.0209	92.4
			Average	90.8
			Standard deviation	1.6

Reaction of 2-phenyl-2,3-dihydro-1H-1,3,2-benzoxazaborole (**2.1**) **and benzene-1,2-diamine** (**2.5**). Benzoxazaborole **2.1** (9.8 mg, 0.05 mmol, 1 equiv) and benzene-1,2-diamine (**2.5**) (5.4 mg, 0.05 mmol, 1 equiv), and $CDCl_3$ (0.7 ml) were combined in NMR tube and the reaction progress was monitored using ^{1}H NMR spectroscopy. The NMR spectrum was obtained soon after mixing, at 1.5h, 24h, and until no further changes were observed (see Figure 14). Partial ^{1}H NMR data (300 MHz, $CDCl_3$): δ 7.92 (d, ArH (**2.1**)), 7.70 (d, ArH (**2.6**)).

$$\text{Percent conversion} = \frac{\text{Integration of (2.6) at } \delta\ 7.70}{\text{Integration of (2.6) at } \delta\ 7..70 + \text{(2.1) at } \delta\ 7.92 + \text{boron-containing intermediates at } \delta\ 8.20} * 100\%$$

Reaction of 2-phenyl-2,3-dihydro-1H-1,3,2-benzoxazaborole (**2.1**) **and 2-(ethylamino)phenol** (**2.7**) Benzoxazaborole 2.1 (9.8 mg, 0.05 mmol, 1 equiv) and 2-(ethylamino)phenol (6.8 mg, 0.05 mmol, 1 equiv), and $CDCl_3$ (0.7 ml) were combined in a NMR tube and the reaction progress was monitored using NMR spectroscopy (Figure 17). This was monitored in three separate trials at the same concentration. There was no difference in the spectra between the first measurement (soon after mixing) and after 0.5h. Partial ^{1}H NMR data (300 MHz, $CDCl_3$): δ 7.92 (**2.1**+**2.8**) (d, ArH), 3.95 (q, CH_2 (**2.8**)), 3.15 (q, CH_2 (**2.7**)), 1.47 (t, 3H, (**2.8**)), 1.27 (t, (**2.7**)).

Percent conversion = $\frac{\text{Integration of } (2.8)\ at\ \delta\ 3.95}{\text{Integration of } (2.7) \text{ at } 3.15 + (2.8)\ at\ \delta\ 3.95} * 100\%$

Table 4. *^{1}H NMR signals and integrations used to determine the percent conversion of 3-(ethyl)benzoxazaborole **2.8**.*

Trial #	Reactant (**2.7**) H_a δ 3.15 (d)	Product (**2.8**) H_b δ 3.95 (d)	Percent conversion (%)
i	0.0765	1.00	92.8
ii	0.0824	1.00	92.3
iii	0.1100	1.02	90.2
		Average	91.8
		Standard deviation	1.3

Computational analysis to show the difference between the solution-phase and gas-phase of molecules of 2-phenyl-2,3-dihydro-1H-1,3,2-benzoxazaborole (**2.1**)**, catechol (2.2), benzodioxaborole 2.3, and 2-aminophenol (2.4) using basis sets 6-311++G(d,p) and 6-311+G(d,p).** The individual free energies of **2.1**, **2.2**, **2.4**, and **2.6** in both chloroform

and gas-phase were calculated and tabulated to check the effect of solvation when using chloroform as a solvent model (see Table 5).

Table 5. *Individual free energy values using basis sets 6-311+G(d,p) and 6-311++G(d,p) in $CHCl_3$ and gas-phase.*

	6-311G+(d,p)			
	$CHCl_3$ (Hartrees)	Gas-phase (Hartrees)	ΔG (Hartrees)	ΔG (kJ/mol)
2.1	-618.244908	-618.238421	-0.006487	-17.0316
2.2	-382.73523	-382.729434	-0.005796	-15.2174
2.4	-362.850907	-362.845308	-0.005599	-14.7002
2.6	-598.356914	-598.350437	-0.006477	-17.0054
	6-311G++(d,p)			
	$CHCl_3$ (Hartrees)	Gas-phase (Hartrees)	ΔG (Hartrees)	ΔG (kJ/mol)
2.1	-618.245002	-618.238580	-0.006422	-16.8609
2.2	-382.735364	-382.729550	-0.005814	-15.2646
2.4	-362.851072	-362.845626	-0.005446	-14.2984
2.6	-598.356880	-598.350606	-0.006274	-16.4723

CHAPTER III

Hydrolysis of Heterobenzoboroles

Computational chemistry is a growing field, which incorporates theoretical models and mathematical functions/algorithms to model the behavior of chemical systems into efficient programs implemented on computers. Contemporary computational chemistry has become an indispensable tool for experimental chemistry, as it can be used to predict properties and examine structures that cannot be achieved experimentally. Moreover, it can be used to compare the properties of structurally analogous molecules (isostructural or isosteric). Examples of such properties are absolute and relative energies, conformations and their relative stabilities, potential energy surfaces (PES), electronic charge density distributions, dipole moments, vibrational frequencies, reactivity, solvation results, or other spectroscopic information. Computational chemistry can be used to examine aspects of a reaction mechanism that cannot be determined experimentally, such as the possible transition states (TS), short-lived intermediate structures, and their absolute and relative energies. This thesis uses computational chemistry to explore the mechanism of formation/hydrolysis of heterobenzoboroles and to compare (support or refute) experimental results.[43]

Previous work

As described in chapters I and II, previous group members have studied the thermodynamic and kinetic nature of heteroboroles such as dioxaborole, 3-(alkyl)benzoxazaborole, and diazaborole using ^{1}H NMR spectroscopy and computational chemistry.[29,38] The equilibrium constants and Gibbs free energy values for the heterobenzoborole exchange were determined by experimental studies and supported by computational calculations.[29,38]

These studies indicated that heterobenzoboroles show different stabilities and rates of exchange.[29,38] Accordingly, the stability of alkyl benzoxazaboroles is similar to benzodioxaborole and roughly an order of magnitude more stable than that of the benzodiazaborole. Further, a rapid interchange was observed between benzodioxaboroles and benzoxazaboroles and apparent equilibrium is achieved at room temperature soon after mixing. In contrast, the interchange between benzodiazaborole and benzoxazaboroles is very slow at room temperature and apparent equilibrium took nearly one week to be established.[29,38] These observations lead us to explore the reasons for differences in the thermodynamic stability and rates of formation and exchange of heteroboroles.

Present study

To explore the reasons for the differences in stability and kinetics of exchange, we initiated the present study into the potential intermediate structures that might exist during the formation/hydrolysis of heteroboroles (see Figure 20 for example) with the expectation of elucidating insight into the mechanism.

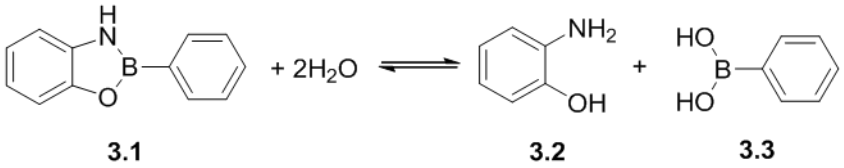


Figure 20. *The hydrolysis (forward reaction) and formation (reverse reaction) of benzoxazaborole* ***3.1***.

Initial proposed mechanism

To begin, a proposed set of intermediates starting from benzoxazaborole **3.1** to products phenylboronic acid (**3.3**), and 2-aminophenol (**3.2**) was examined computationally. The borole ring of benzoxazaborole is asymmetric; therefore, the hydrolysis of benzoxazaborole may involve two potential pathways (see Figure 21). Path A where the boron-nitrogen bond breaks during the ring-opening step giving rise to intermediate A or path B where the boron-oxygen bond breaks during the ring-opening step resulting in intermediate B.

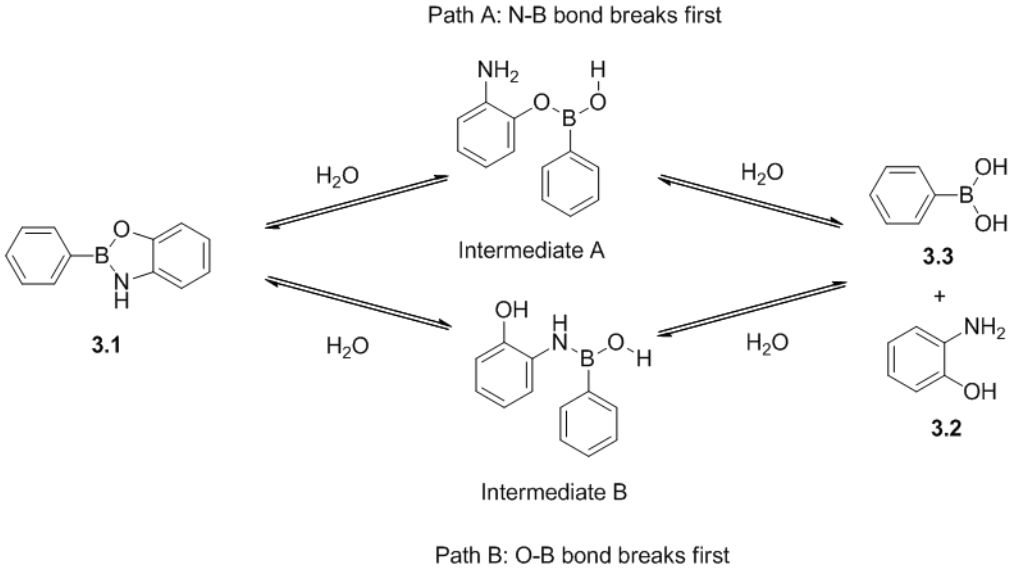


Figure 21. *Two potential pathways for benzoxazaborole hydrolysis.*

A more detailed scheme of potential intermediates (nine structures for each pathway) for the hydrolysis of benzoxazaborole is shown in Figure 22. The initial step is the coordination of a water molecule to the boron in benzoxazaborole **3.1A** (the complex is referred to as **3.4**). The formation of this bond results in a negative charge on boron and a positive charge on the oxygen of the water molecule. The next step involves a proton transfer from the oxygen to either the nitrogen (Path A) or the oxygen (Path B). In path A,

the NH group on the borole ring accepts a proton and becomes cationic (**3.6A**), similarly, in path B, the oxygen in the borole ring accepts a proton to become cationic (**3.6B**). Due to the instability of positive charge on electronegative atoms such as nitrogen and oxygen, either the B-N bond or B-O bond undergoes heterolysis to intermediates **3.7A** or **3.7B**, respectively. Next, a second water molecule coordinates to intermediate **3.7A** or **3.7B** to give structures **3.8A** or **3.8B**, respectively. After a series of proton transfers to get structures **3.10A**/**3.10B** a final heterolysis step will result in the products, phenylboronic acid (**3.3**) and 2-aminophenol (**3.2**).

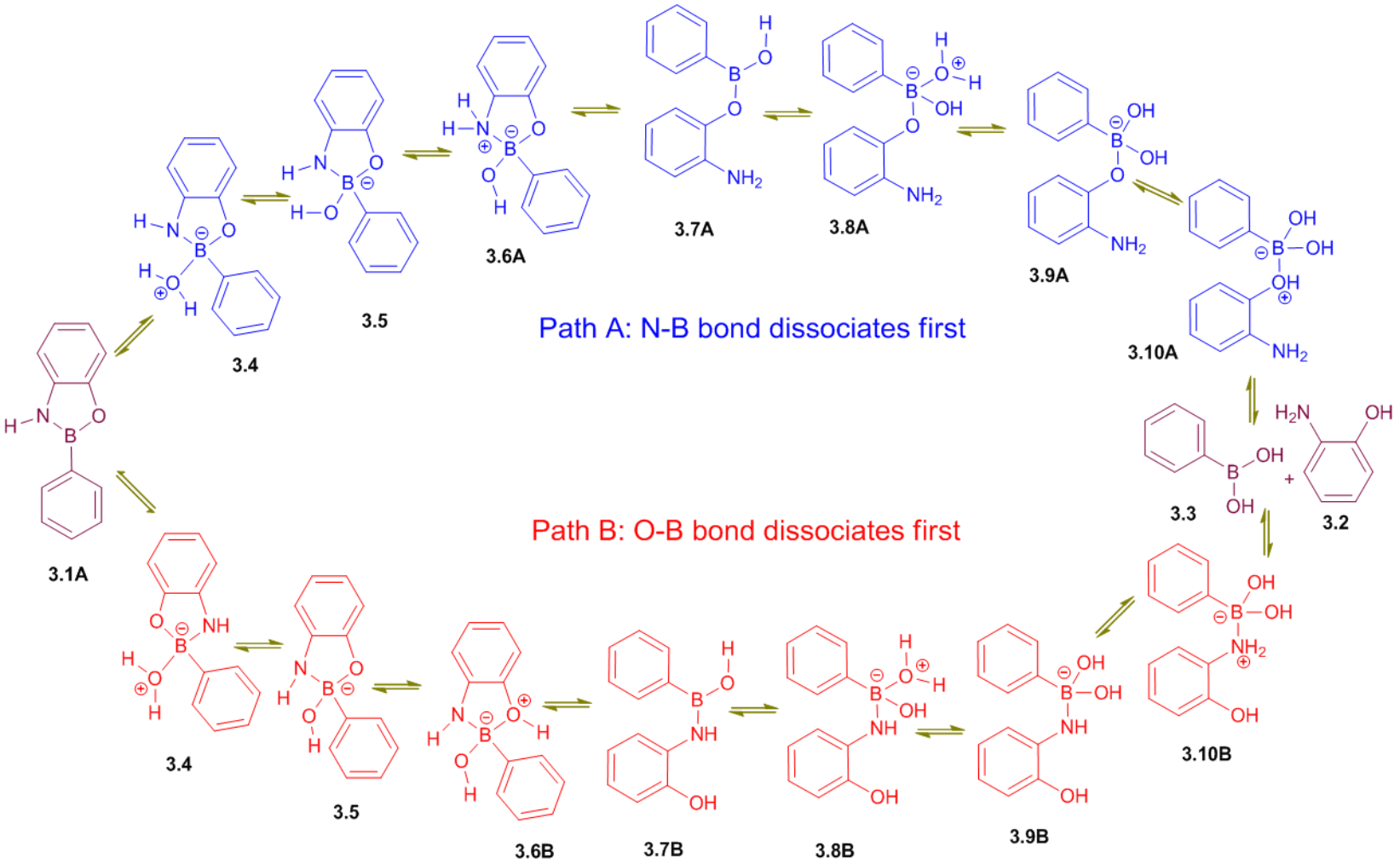
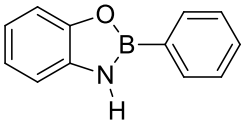
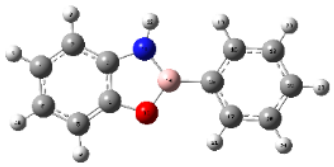
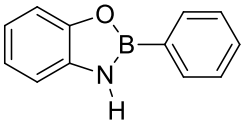
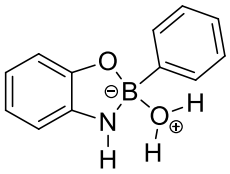
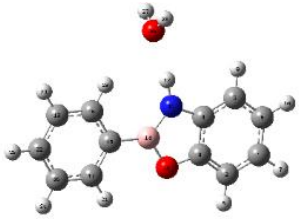
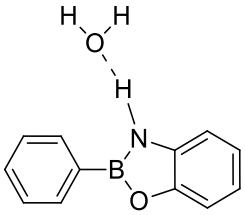
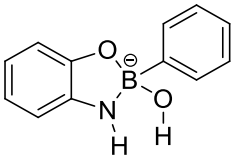
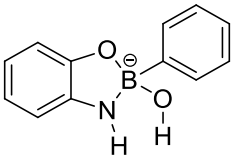
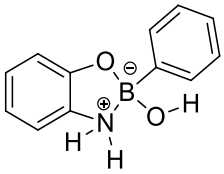
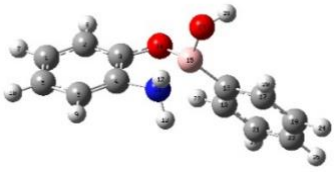
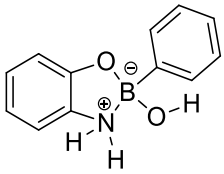
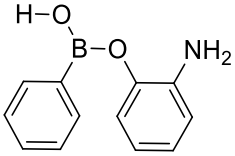
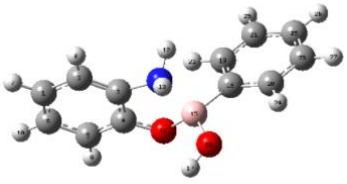
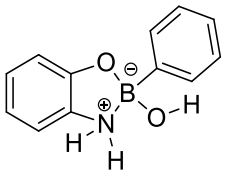
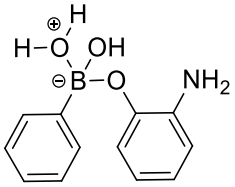
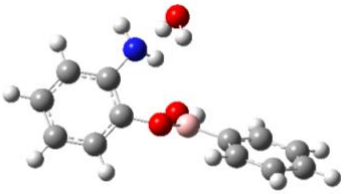
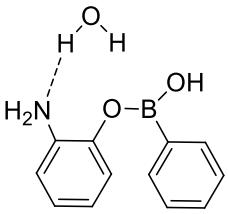


Figure 22. *Proposed intermediates during the hydrolysis of benzoxazaborole. Top: Path A, N-B bond breaks first. Bottom: Path B, O-B bond breaks first.*

The structures of the supposed reactants, products, and intermediates were built in GaussView 5.0.9 and subjected to geometry optimization and frequency calculations using Gaussian G09W software. These calculations were performed using DFT with the B3LYP functional and the 6-311G+(d,p) basis set with chloroform as the solvent model.[40] Initially, the Gibbs free energy of the overall reaction ΔG(reaction) was determined using the equation ΔG(reaction) = G(products)-G(reactants) (see Figure 20). The ΔG for hydrolysis of benzoxazaborole was found to be endergonic (20.65 kJ/mol).

In addition to the reactants and products, we looked at the geometry optimization of the 7 proposed intermediates of path A. Table 6 includes the predicted and geometry optimized structures. Upon inspection of the structures in Table 6, only 5 of the 9 agreed with the initial predictions. These include benzoxazaborole **3.1**, products (**3.2** and **3.3**), and intermediates **3.5**, **3.7A,** and **3.9A**. The remaining predicted structures (**3.4**, **3.6A**, **3.8A**, and **3.10A**) did not give the expected result. The structures involving the coordination of water to the boron of the benzoxazaborole (**3.4** and **3.8A**, respectively) formed hydrogen bonds instead of coordinating to the boron. This was determined by measuring the relevant interatomic distances. In hydrogen-bonded **3.4**, the corresponding bond distances were 3.99 Å for B(borole)···O(H_2O) and 1.97 Å for O(H_2O)···H(N-H of borole). Further, the interatomic distances of **3.8A** were 4.50 Å B(**3.7A**)···O(H_2O) and 1.95 Å for N(**3.7A**)···H(H_2O). This problem was overcome in future calculations by choosing a different functional.

Table 6. *Predicted and geometry-optimized structures during the hydrolysis of benzoxazaborole* ***3.1*** *at DFT/B3LYP/6-311+G(d,p)/$CHCl_3$.*

Index	Originally predicted structure	Geometry-optimized output file	Geometry-optimized structure
3.1			
3.4			
3.5			
3.6A			
3.7A			
3.8A			

(continued)

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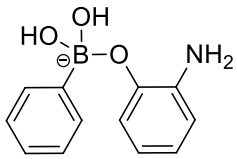
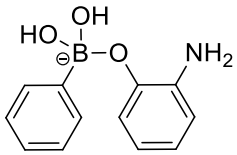
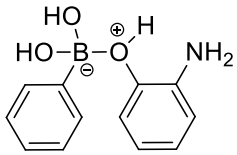
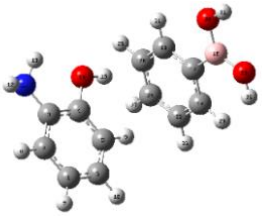
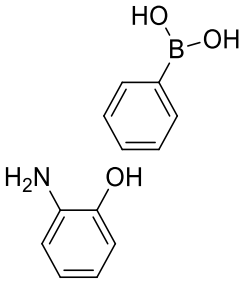
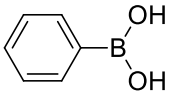
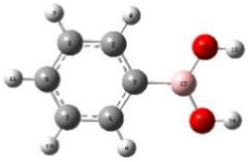
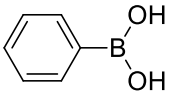
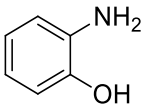
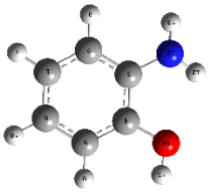
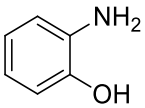
3.9A			
3.10A			
3.3			
3.2			

More interestingly, the input structures for **3.7A** converged to **3.6A**, and models for **3.10A** converged to **3.2** and **3.3** upon geometry optimization. This result caused us to reevaluate our proposed mechanism. Additionally, since intermediates **3.5** and **3.9A** are higher energy structures due to the negative charge on the boron and should be balanced with a counter ion, we decided not to include them in the subsequent analysis. The newly proposed mechanism involves two main steps. In step one, water is added across the B-X bond of the borole ring through a transition state (**TS1**) to give an intermediate (**3.7**). In

step two, a second water molecule adds across the B-X' bond, which goes through a second transition state (**TS2**) to form the products (**3.2** and **3.3**) (Figure 23). This pathway involves 5 structures in total, including the starting borole (**3.1**), water coordinated to borole (**3.4**), intermediate (**3.7**), water coordinated intermediate (**3.8**), and the products (**3.2** and **3.3**). This alternative mechanism is similar to a recently reported study on the hydrolysis mechanism of COFs.[39] The authors of this report also used a lower level of theory and a different basis set, which we have adopted for the remainder of our calculations.

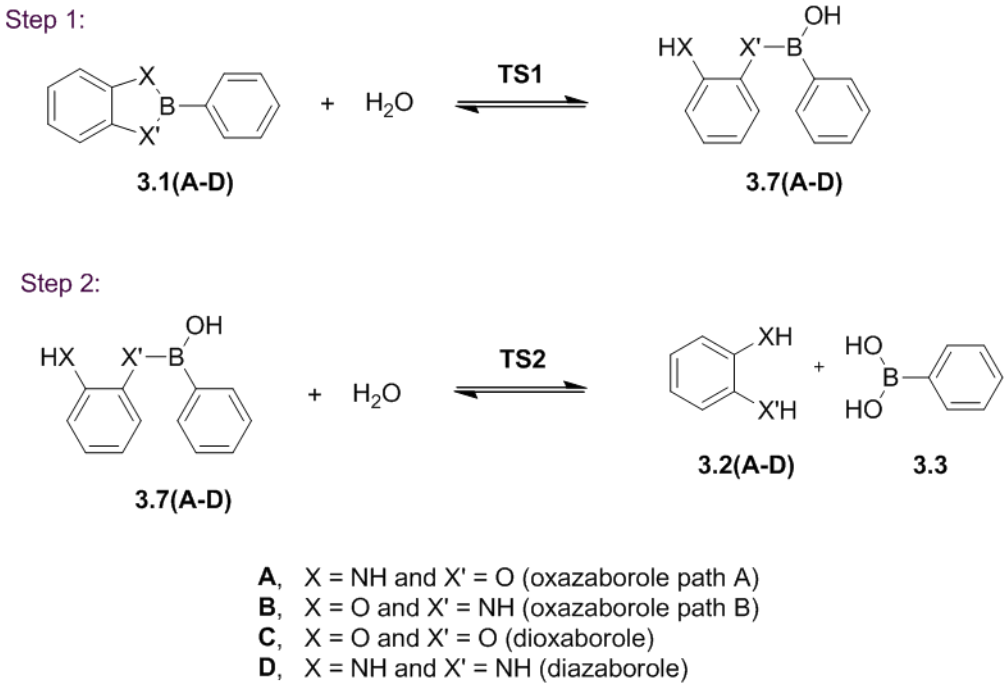


Figure 23. *Proposed steps for the hydrolysis of benzoboroles **3.1A-D**.*

Methodology

Gaussian G09W software was used to carry out all computational calculations. Geometry optimizations and frequency calculations were performed in the gas phase at the density functional theory (DFT) level using the long-range corrected ω-B97XD functional and the 6-31G(d,p), double zeta basis set.[39] The zero-point corrected sum of electronic and thermal free energies were used as the thermochemistry data to calculate and analyze the changes

in energies during each step. The Synchronous Transit-Guided Quasi-Newton (STQN) QST3 algorithm[44] was employed to locate estimates for the transition states (TS), which were identified by confirming that they have a single imaginary frequency with the corresponding eigenvector pointing toward the reactants/products.[44] Furthermore, the intrinsic reaction coordinate (IRC)[45,46] calculation was performed to ensure that the optimized TS is connected to the two relevant minima (reactants and products).[46] Both the QST3 algorithm and the IRC calculations were performed at the same level of theory and the basis set.

A transition state (TS) is a molecular entity that has a lifetime no longer than a bond vibration cycle and exhibits some structural characteristics of both the reactants and the products. The TS can be better identified through the energy profile diagram. Transition states are local energy maximums and have a partial bond character. The STQN method is used for locating transition structures computationally. This method was introduced by H. B. Schlegel and coworkers.[44] The quadratic synchronous transit (QST) approach is performed to get closer to the quadratic region of the transition state (TS) and then uses a Quasi-Newton or eigenvector-following algorithm to complete the optimization. The QST method searches for a maximum along an arc connecting reactants and products and for a minimum in all directions perpendicular to the arc. The STQN method has two main approaches to locate the TS, QST2, and QST3. The QST2 method requires two structures, reactants, and products as its input, while the QST3 method requires the reactant, product, and an initial guess of the transition state.[44]

The reaction path can be defined as the curve on the potential energy surface connecting the reactants and products through the transition state.[45] This is a useful

theoretical tool to study chemical reactions using the "potential energy surface" of the reacting system.[2] The intrinsic reaction coordinate (IRC) is used to confirm that the transition state is connected to reactants and products by following the path of separate descent forward and backward from the saddle point (or transition state) to the products and reactant, respectively.[38]

Relative to other functionals, ω-B97X-D is significantly better for nonbonded interactions, and it gives similar outcomes for the covalent interactions.[47] When comparing the long-range corrected *ω*-B97X-D functional with the well-established DFT-D functionals (B97-D, B3LYP-D and BLYP-D), the ω-B97X-D functional is considered to be superior in overall performance including calculating atomization energies, reaction energies, non-covalent interaction energies, equilibrium geometries, and a charge-transfer excited states, and ω-B97X-D shows improvement over other empirical dispersion-corrected density functionals, while for covalent systems and kinetics it performs noticeably better.[47]

Due to the higher symmetry of benzodioxaborole (**3.1C**) and literature precedent,[39] we chose to test this methodology on this system. In the first step, a water molecule coordinates to the boron-oxygen bond and reacts to form an intermediate structure (which we refer to as **3.7C** see Figure 24). In the second step, **3.7C** reacts with another molecule of water, which generates phenylboronic acid (**3.3**) and catechol (**3.2C**). Each step has a transition state, labeled as **TS1-C** and **TS2-C**, respectively (Figure 24).

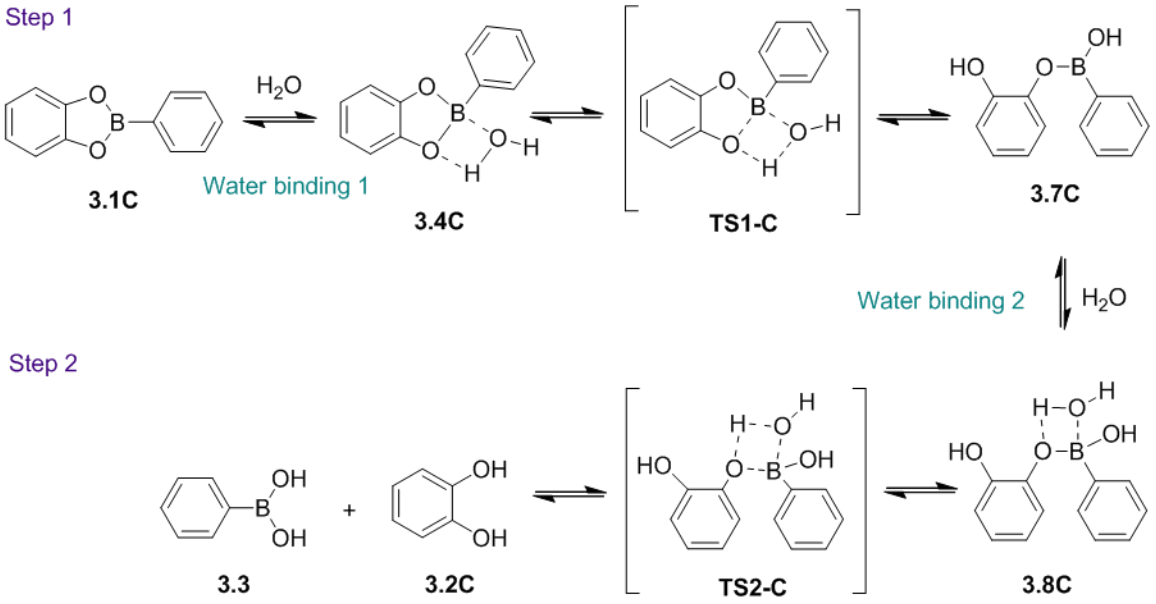


Figure 24. *Proposed mechanism for the hydrolysis of dioxaborole **3.1C**.*

The binding of a water molecule allows the [B(**3.1C**)···O(H_2O)] and the O(**3.1C**)···H–O(H_2O) interaction giving rise to the water coordinated benzodioxaborole **3.4C**, as displayed in Figure 25. The binding energy (E_b), $E_b = E_{(3.4C)} - (E_{(Isolated\ 3.1C)} + E_{(H2O)})$ of this interaction was calculated to be 6.7 kJ/mol. Moreover, the binding of the water molecule weakens the B–O bond of **3.1C**, as it elongates from 1.380 Å to 1.392 Å (Figure 25). Dissociation of the B–O bond results in intermediate **3.7C** (see Figure 26).

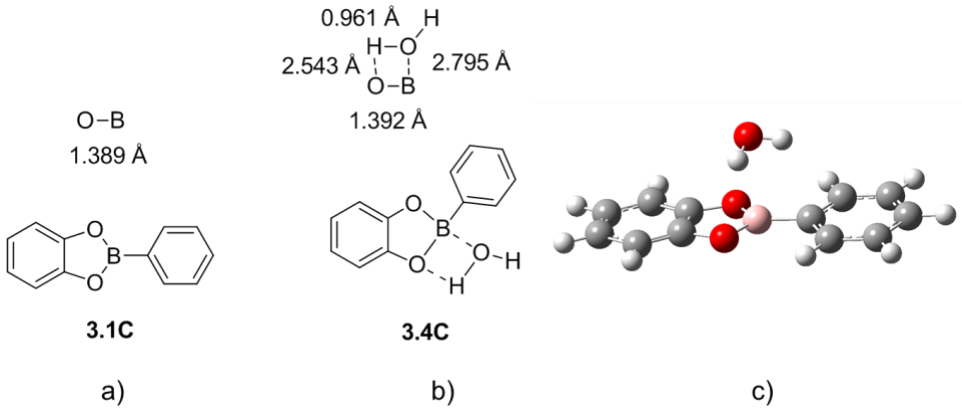


Figure 25. *Illustrated interatomic distances for a) unbound **3.1C**, b) water coordination to benzodioxaborole (**3.4C**), and c) geometry-optimized **3.4C**.*

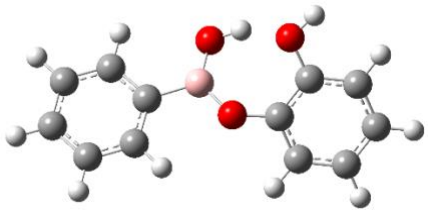


Figure 26. *Geometry-optimized intermediate **3.7C**.*

Using **3.4C** as the reactant, **3.7C** as the product, and an initial guess of the transition state, the optimized structure for the transition state (**TS1-C**) was obtained by the QST3 algorithm. The corresponding **TS1-C** and the relevant interatomic distances are shown in Figure 27. The energy barrier (**TS1-C**) of this ring-opening step (**3.4C→3.7C**) was determined to be 109.60 kJ/mol.

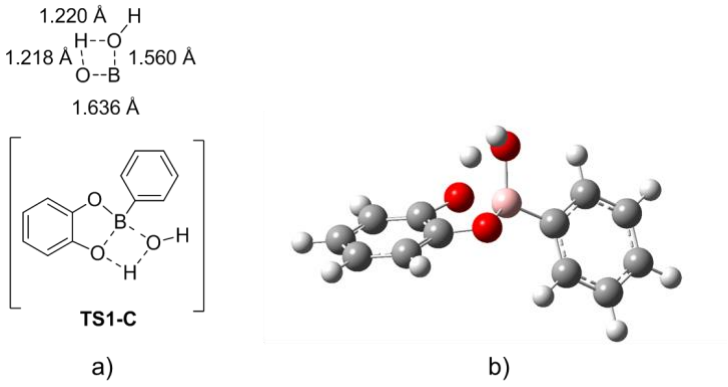


Figure 27. *QST3 output for the transition state **TS1-C**. a) relevant interatomic distances and b) output structure.*

Furthermore, the Intrinsic Reaction Coordinate (IRC) calculation of the benzodioxaborole hydrolysis was performed to ensure that **TS1-C** is connected to two relevant minima (**3.4C** and **3.7C**). The calculations were performed for both directions, forward and reverse, having 15 steps each. The corresponding IRC calculations (IRC1) indicated that the **TS1-C** is connected to **3.4C** as the reactant and **3.7C** as the product. Figure 28 displays the total energy along the IRC pathway, and according to Figure 27, it is clear that **TS1-C** is a maximum along the reaction coordinate.

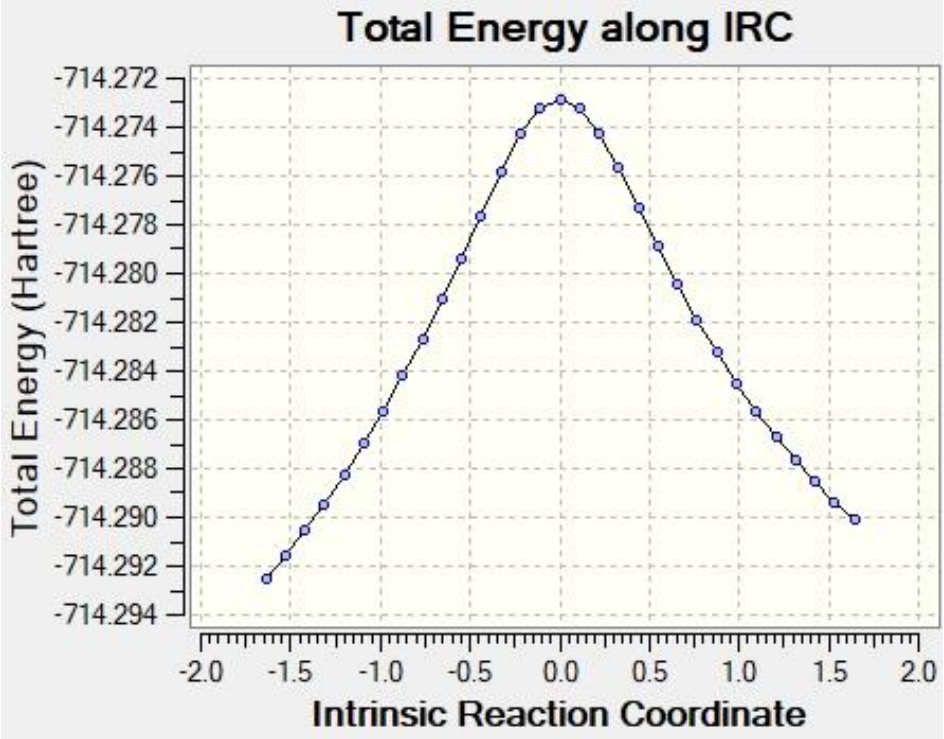


Figure 28. *The result of the IRC1 calculation during the first step of benzodioxaborole hydrolysis.*

In the second step, a second water molecule coordinates to the remaining B–O bond of **3.7** to give the bound structure **3.8C**, (see Figure 29b), and the binding energy (E_{b2}) was found to be 8.86 kJ/mol. The second boronate ester bond dissociation was studied according to the QST3 algorithm, and the corresponding transition state (**TS2-C**) was found by using a guess for **TS2-C**, along with **3.8C** and **3.2C·3.3** as the reactant and product, respectively (see Figure 29). The energy barrier (**TS2-C**) of the second boronate ester bond dissociation (**3.8C→3.2C·3.3**) was found to be 91.58 kJ/mol (see Figure 30).

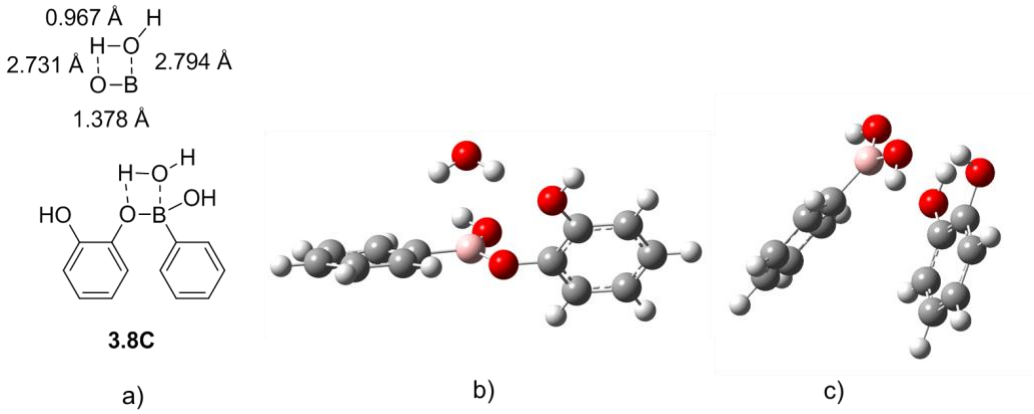


Figure 29. *a) Relevant interatomic distances of water coordinated intermediate (**3.8C**), b) geometry-optimized output structure for **3.8C**, and c) geometry-optimized output structure for the phenylboronic acid-catechol (**3.2C·3.3**) coordinated structure*.

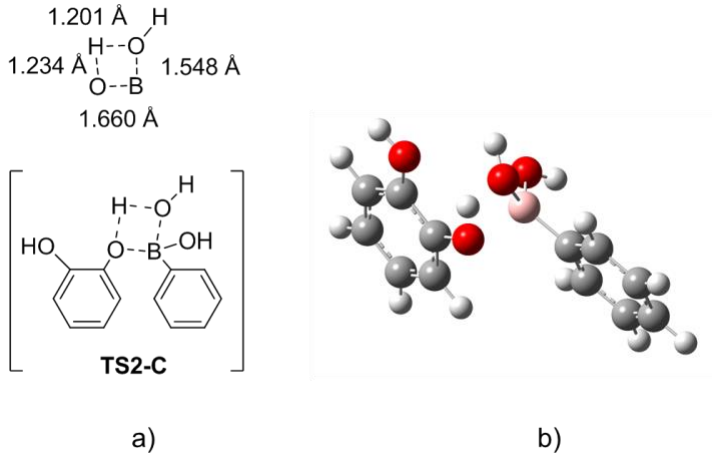


Figure 30. *QST3 output for the transition state **TS2-C**. a) relevant interatomic distances and b) output structure.*

To check the reproducibility of the **TS** obtained from the QST3 algorithm and the IRC calculation, the below-mentioned steps were followed (see Figure 31). We chose the second step during the hydrolysis of **3.1C** for this follow-up study. The QST3-I calculation was performed using the previously geometry optimized structures **3.8C** and **3.2C·3.3**, and

the initial guess for **TS2-C**. The outcome of QST3-I, **TS2-C** (we will call this **TS2-I**) was subjected to IRC-I to ensure it was connected to relevant minima, which were the reactant (**3.8C**) and the product (**3.2C·3.3**). The IRC-I results for the coordinated **3.2C·3.3** structure displayed a slight difference compared to its geometry-optimized structure. This observation led us to calculate the energy of the structures that resulted from IRC-I. There was a 53.70 kJ/mol difference between IRC-I results and the geometry-optimization results of the **3.8C**, and a 78.68 kJ/mol difference for the **3.2C·3.3** coordinated structure (see Table 7). To ensure the accuracy of this transition state result, a similar QST3 calculation (QST3-II was conducted using **TS2-I** and the geometry optimized output structures of IRC-I. The new **TS2-II** was compared structurally with **TS2-I** and the energy difference was checked for each **TS** (Figure 31). There was no difference between the absolute energy of **TS2-C-I** and **TS2-C-II**. Once the energies were compared with the originally geometry-optimized structures and recycled structures from the IRC-I, there was a 3.05 kJ/mol difference between the first geometry-optimized **3.8C** and the second optimized **3.8C**. Similarly, a 3.68 kJ/mol difference has been seen for the original and second optimized **3.2C·3.3** structure. Even though output for the IRC has different (higher) energies when it recycled back to the QST3 calculation similar results were obtained for the **TS**. This study provides evidence that the **TS** obtained by the QST3 algorithm is accurately connected to its relevant minima.

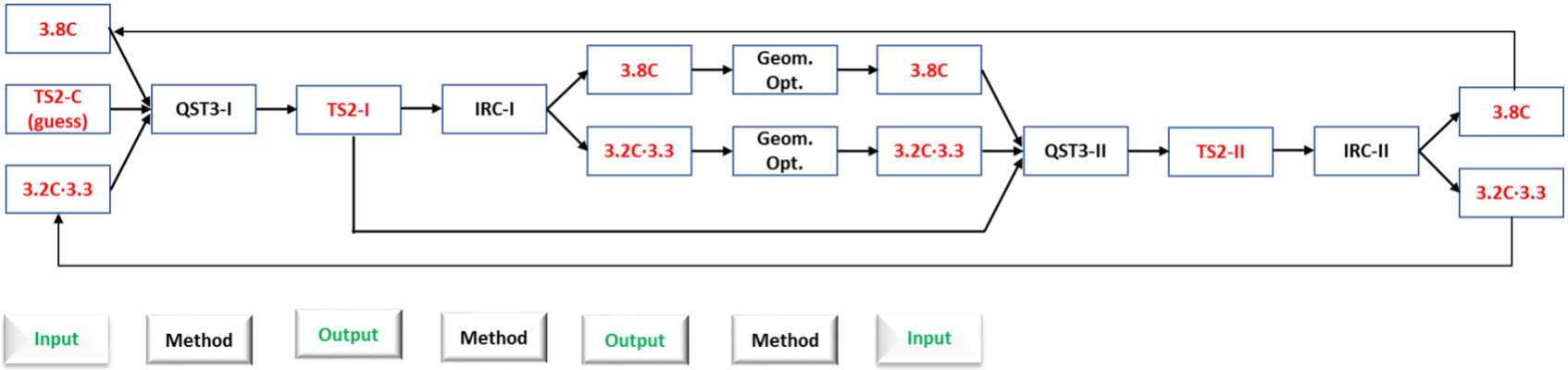


Figure 31. *Schematic diagram showing steps for QST3 and IRC method confirmation*.

Table 7. *Energy values of QST3 and IRC calculations (all values are in kJ/mol and relative to **3.8C**).*

Structure	Geometry optimized (Input)	QST3-I result	IRC-I result	IRC-I result (Geometry optimized)	QST3-II result	IRC-II result	IRC-II result (Geometry optimized)
3.8C	0	-	53.70	3.05	-	53.70	3.04
TS2-C	-	91.58	-	-	91.58	-	-
Bound **3.2C·3.3**	-24.50	-	78.68	-3.68	-	78.68	-3.63

Once the mechanism and intermediates of the hydrolysis of benzodioxaborole were more understood, we turned our attention to the hydrolysis of benzoxazaborole, which was studied using the same computational method. As illustrated in Figure 21 because of the asymmetric nature of the borole ring, the hydrolysis of benzoxazaborole may involve two potential pathways path A and path B.

In the first step of path A, water is added across the boron-nitrogen bond of **3.1A**. This involves the B(**3.1A**)···O(H_2O) and N(**3.1A**)···H(H_2O) interaction to form the water coordinated benzoxazaborole (**3.4A**). The binding energy (E_{b1}) for this interaction was calculated to be 18.33 kJ/mol (see Figure 32).

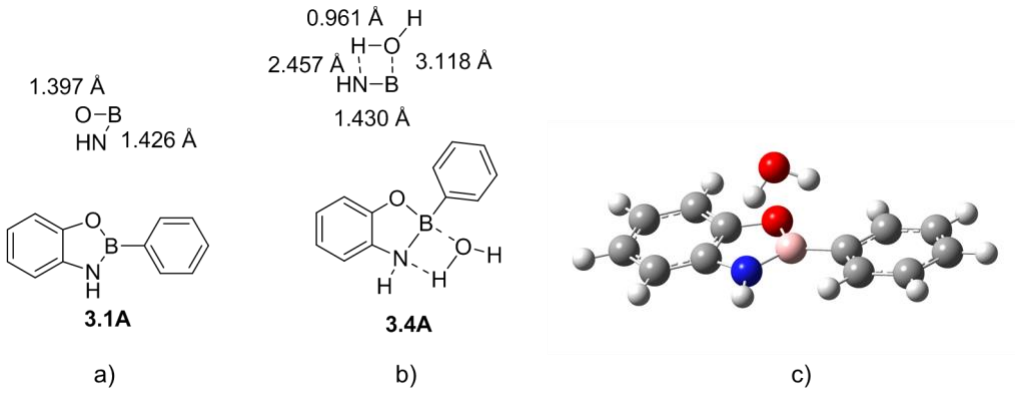


Figure 32. *Illustrated interatomic distances for a) unbound **3.1A**, b) water coordinated **3.4A**, and c) geometry-optimized output of water coordination to benzodioxaborole (**3.4A**).*

Moreover, the binding of the water molecule weakens the B–N(H) bond of **3.1A**, through the energy barrier related to transition state (**TS1-A**) the coplanar five-membered borole ring opens and forms the intermediate (**3.7A**). The associated energy barrier **TS1-A** (see Figure 33) of the boronate ester bond dissociation (**3.4A→3.7A**) is calculated to be 91.46 kJ/mol. The intermediate **3.7A** has a 5-membered ring assembly having the

dissociated NH_2 group coordinated with B(borole) after geometry optimization (see Figure 34).

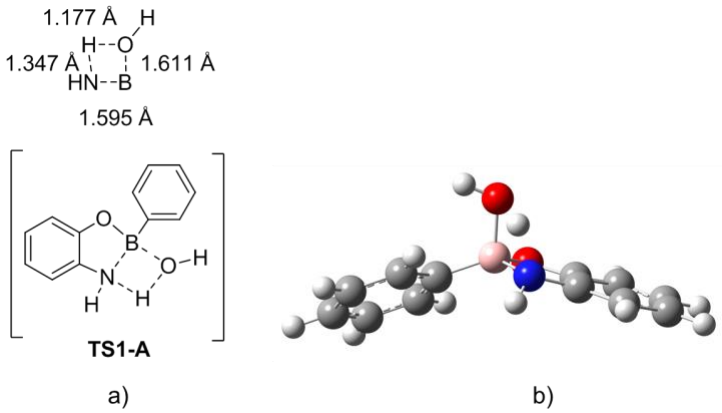


Figure 33. *QST3 output for the transition state* ***TS1-A****. a) relevant interatomic distances and b) output structure.*

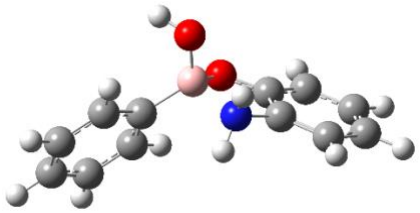


Figure 34. *Geometry-optimized intermediate* ***3.7A***.

In the second step, a second water molecule is added across the remaining B–O bond, B(**3.7A**)···(O)(H_2O) to form a water-coordinated intermediate (**3.8A**) (Figure 35). The binding energy (Eb_2) for the interaction was found to be -13.99 kJ/mol. The corresponding transition state (**TS2-A**) was obtained using a guess for **TS2-A**, along with **3.8A** and **3.2A·3.3** as the reactant and product, respectively (see Figure 35). The energy barrier (**TS2-A**) of the B-O bond dissociation (**3.8A→3.2A·3.3**) to form the products,

phenylboronic acid, and 2-aminophenol **3.2A·3.3**, was found to be 113.80 kJ/mol (Figure 36).

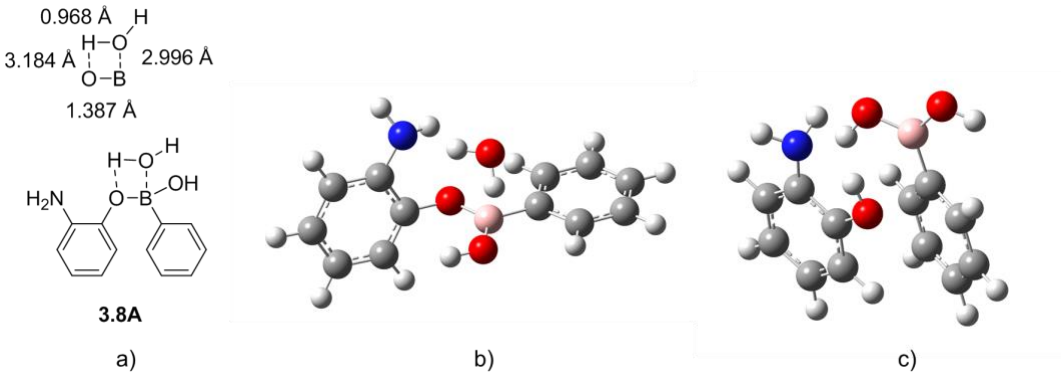


Figure 35. *a) Relevant interatomic distances of water coordinated intermediate (**3.8A**), b) geometry-optimized output file of **3.8A**, and c) geometry-optimized output file of coordinated products **3.2A 3.3**.*

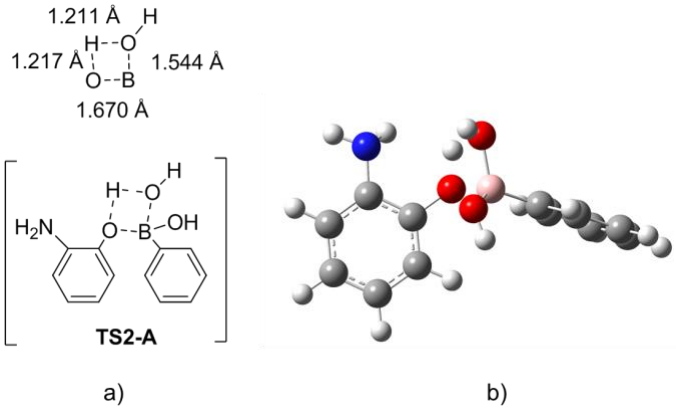


Figure 36. *QST3 output for the transition state **TS2-A**. a) relevant interatomic distances and b) output structure.*

In path B water coordinates to the boron of the borole ring, O(H_2O)···B(**3.1A**), resulting in water coordinated four-membered ring (**3.4B**) (see Figure 37). The binding energy (E_{b1}) for this interaction was calculated to be 13.10 kJ/mol.

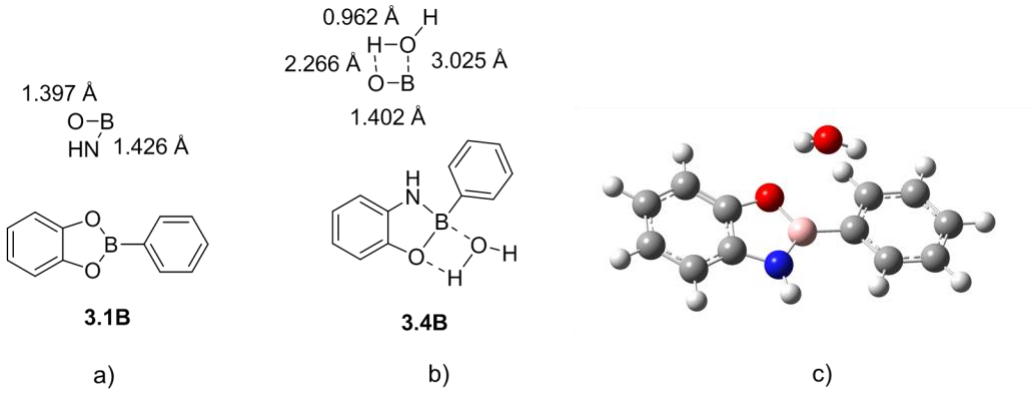


Figure 37. *Illustrated interatomic distances for a) unbound **3.1B**, b) water coordinated **3.4B**, and c) geometry-optimized output of water coordination to benzoxazaborole (**3.4B**).*

The corresponding transition state (**TS1-B**) of the boronate ester bond dissociation (**3.4B→3.7B**) is calculated to be 126.54 kJ/mol (see Figure 38). The resulting intermediate (**3.7B**) has a seven-membered ring structure, similar to the intermediate during the hydrolysis of **3.1C**, having a hydrogen bond between the phenol OH group and the oxygen bonded to the boron (Figure 39).

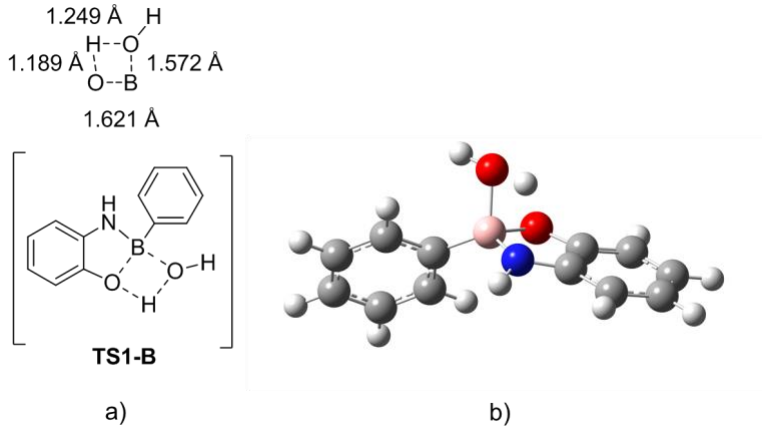


Figure 38. *QST3 output for the transition state **TS1-B**. a) relevant interatomic distances and b) output structure.*

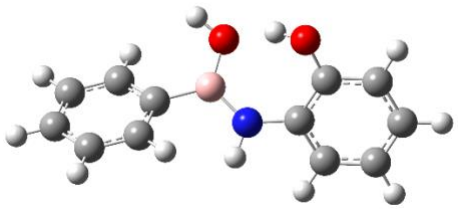


Figure 39. *Geometry-optimized intermediate **3.7B**.*

The addition of a second water molecule to **3.7B** forms the water coordinated intermediate **3.8B,** and the binding energy (Eb_2) for the interaction was found to be 15.53 kJ/mol (Figure 40). Through transition state 2 (**TS2-B** Figure 41) the remaining B-N bond breaks to form the products, phenylboronic acid and 2-aminophenol (**3.2·3.3**), which are the same as seen in path A. The energy barrier for the above step (**3.8B→3.2·3.3**) was found to be 93.21 kJ/mol.

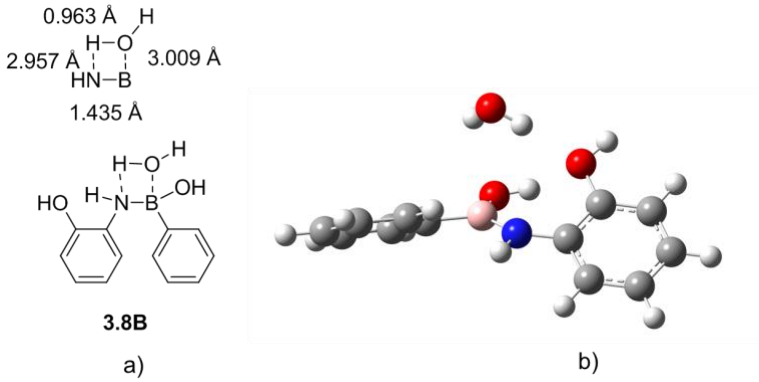


Figure 40. *Relevant interatomic distances of water coordinated intermediate (**3.8B**) and b) geometry-optimized output file of **3.8B**.*

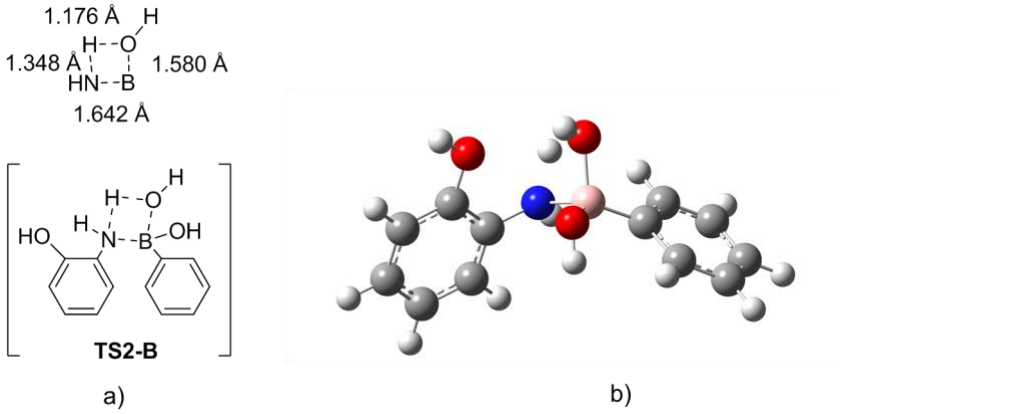


Figure 41. *QST3 output for the transition state* ***TS2-B****. a) relevant interatomic distances and b) output structure.*

Similar to path A of the hydrolysis of benzoxazaborole, water coordinates to the B-N bond of benzodiazaborole (**3.1D**), to form a water coordinated four-membered ring benzodiazaborole (**3.4D**). The binding energy (Eb_1) was calculated to be 10.58 kJ mol^{-1} (see Figure 42).

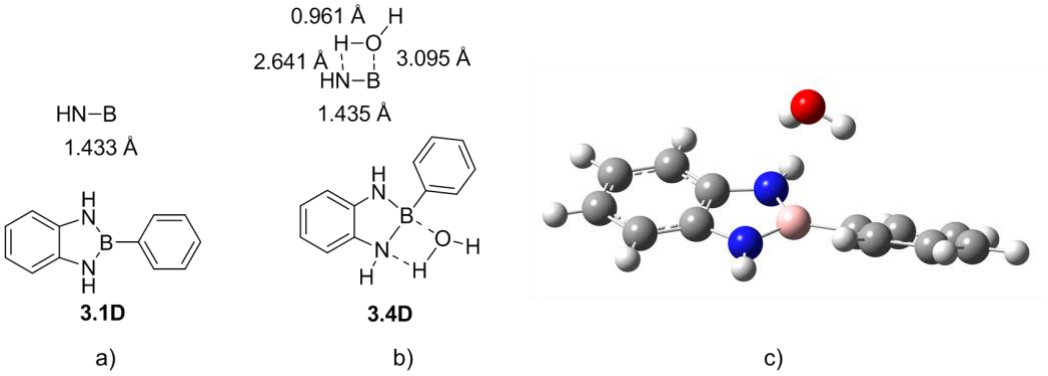


Figure 42. *Illustrated interatomic distances for a) unbound* ***3.1D****, b) water coordinated* ***3.4D****, and c) geometry-optimized output of water coordination to benzodioxaborole* ***(3.4D)****.*

The binding of the water molecule weakens the B–N(H) bond of **3.1D**, through the energy barrier related to transition state (**TS1-D**) the coplanar five-membered borole ring

opens and forms the intermediate (**3.7D**). The relevant energy barrier, transition state 1, **TS1-D** (see Figure 43) (**3.4D→3.7D**) was found to be 115.09 kJ/mol. The associated interatomic distances and output structure from Gaussian are shown in Figure 43. In addition, the intermediate (**3.7D**) shows 5 membered ring structures, which have the nitrogen of the dissociated NH_2 group coordinated to boron after geometry optimization (see Figure 44).

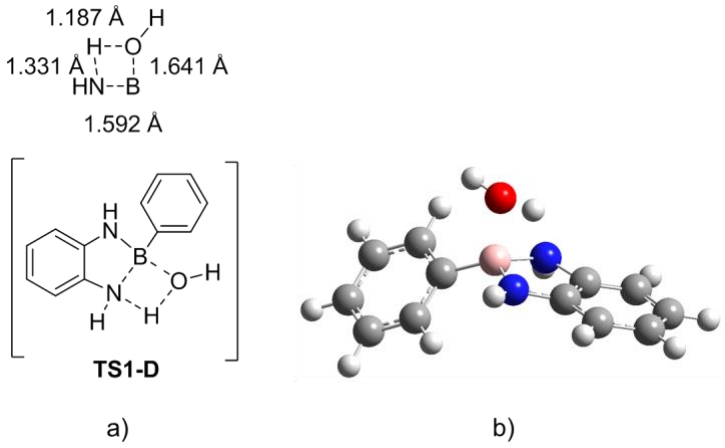


Figure 43. *QST3 output for the transition state **TS1-D**. a) relevant interatomic distances and b) output structure.*

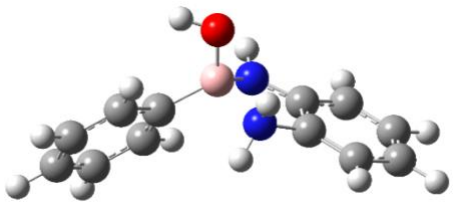


Figure 44. *Geometry-optimized intermediate* **3.7D**.

In the following step, the addition of a second water molecule to **3.7D** forms the water coordinated intermediate **3.8D**, the binding energy (Eb_2) for the interaction was found to be -37.67 kJ/mol. The corresponding transition state (**TS2-D**) was obtained using

a guess for **TS2-D**, along with **3.8D** and **3.2D·3.3** as the reactant and product, respectively (see Figure 45).

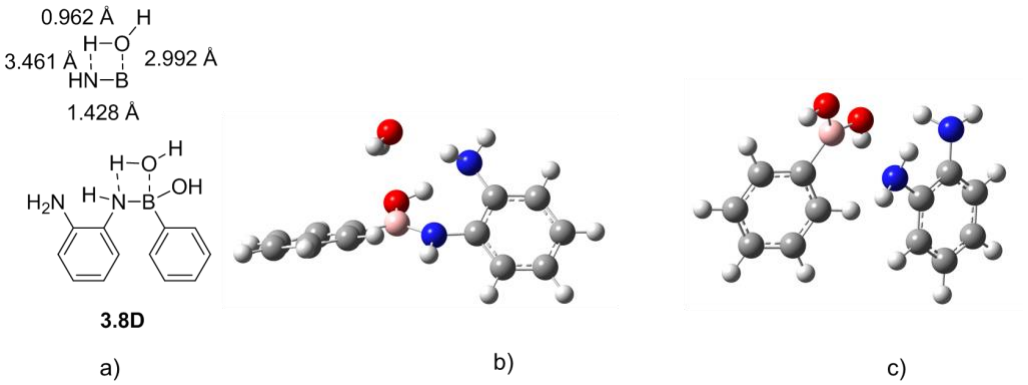


Figure 45. *a) Water coordinated **3.7D**, b) geometry-optimized output structure of **3.8D**, c) **3.2D·3.3** coordinated structure as the product.*

Through the transition state **TS2-D**, the remaining B-N bond dissociates to form the products: phenylboronic acid (**3.2**) and benzene-1,2-diamine (**3.2D**). The energy barrier (**TS2-D**) (see Figure 46) for the above step (**3.8D→3.2D·3.3**) was found to be 104.44 kJ/mol.

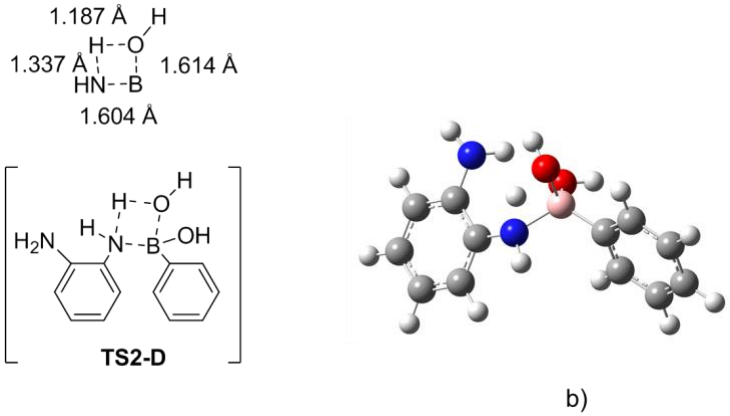
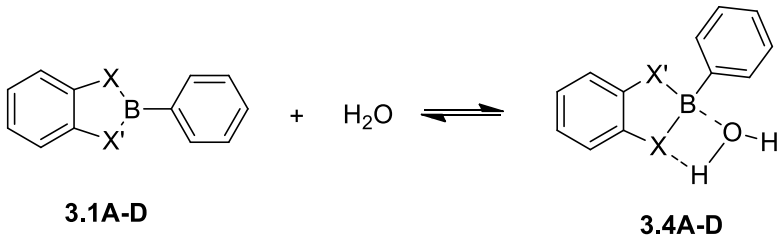


Figure 46. *QST3 output for the transition state **TS2-D**. a) relevant interatomic distances and b) output structure.*

The reactant molecule, **3.8D**, used to obtain **TS2-D** displayed hydrogen bond formation with H(H_2O)···N(NH_2)(**3.2D**) instead of coordinating to the N(N-B(**3.1D**)) (see Figure 45). To validate the output transition state (**TS2-D**), we performed a calculation, similar to the method validation to confirm the legitimacy of the structure of the **3.8D** complex. Therefore, the output structures from the IRC were recycled back to perform a new QST3 calculation, and we saw similar results for both QST3 calculations. Additionally, to confirm **TS2-D**, a QST2 calculation was also performed using the output file of IRC2 the resulting structures (reactant and product). Both QST2 and QST3 calculations had similar frequency/free energy results for **TS2-D**, the difference between free energies was found to be 5.25 x 10^{-3} kJ/mol. In addition, the interatomic distances around the boron of each transition state were observed. A slight difference was observed for interatomic distances of H(H_2O)···N(NH_2), H(H_2O)···O(H_2O), and H(H_2O)···B of **TS2-D** when using QST3 and QST2 methods (see Appendix section).

Water-coordination 1

In the proposed mechanism, the first step involves water-coordination across the B-X bond of the heteroborole **3.1** to form water-coordinated benzoborole **3.4** (see Figure 47). The results of the geometry-optimization of unbound benzoboroles **3.1** and water coordinated benzoboroles **3.4** were observed (see Figure 48), the geometry optimized structures of **3.4** exhibit distorted trigonal planar geometry around the boron atom during water coordination. Moreover, the binding of the water molecule weakens (see Table 8 below) and elongates the B–X bond and slightly shortens the B-X' bond for all heteroboroles (see Table 8).



3.1A-D **3.4A-D**

A, X = NH and X' = O (oxazaborole path A)
B, X = O and X' = NH (oxazaborole path B)
C, X = O and X' = O (dioxaborole)
D, X = NH and X' = NH (diazaborole)

Figure 47. *Water coordination to heteroboroles **3.1A-D**.*

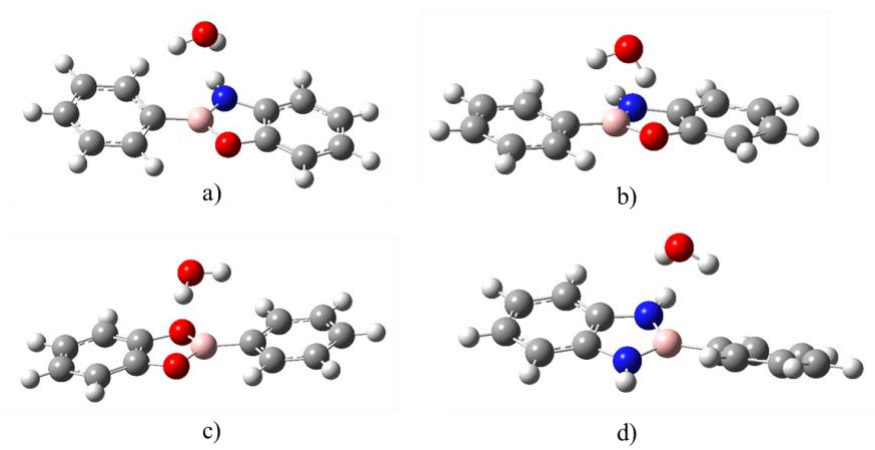


Figure 48. *Geometry-optimized water coordinated structures of a) benzoxazaborole-H_2O (**3.4A**), b) benzoxazaborole-H_2O (**3.4B**), c) benzodioxaborole-H_2O (**3.4C**), and d) benzodiazaborole-H_2O (**3.4D**).*

The IRC output structures for the water coordinated heteroborole **3.4** as the reactant was compared with the originally geometry optimized structure of **3.4**. The structures show different bond lengths (see Table 8), and the geometry around the boron exhibits a more tetrahedral geometry in the IRC output structures (see Figure 49). Moreover, the IRC output files for reactants and products have higher energy values compared with their geometry-optimized structures, indicating that they may not be at a true minimum.

However, similar results for transition states were obtained once those structures from IRC were recycled back to perform a QST3 calculation.

Table 8. *The associated bond lengths of geometry-optimized structures of unbound **3.1** and water-coordinated heterobenzoborole **3.4**.*

Heterobenzoborole	Geometry optimized structure				IRC output	
	3.1		**3.4**		**3.4**	
	Bond lengths (Å)					
	B-X	B-X’	B-X	B-X’	B-X	B-X’
A	1.42	1.39	1.43	1.39	1.52	1.42
B	1.39	1.42	1.40	1.42	1.50	1.46
C	1.38	1.39	1.39	1.38	1.50	1.43
D	1.43	1.43	1.44	1.42	1.52	1.46

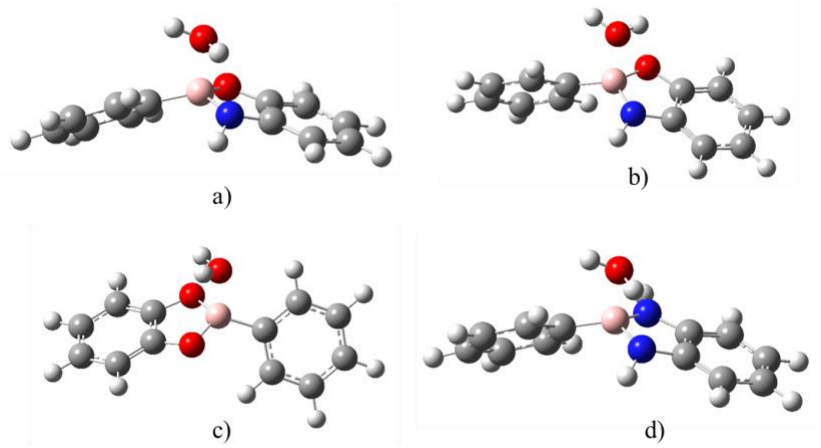


Figure 49. *The structures from the IRC output file. a) benzoxazaborole-H_2O (**3.4A**), b) benzoxazaborole-H_2O (**3.4B**), c) benzodioxaborole-H_2O (**3.4C**), and d) benzodiazaborole-H_2O (**3.4D**).*

Water-coordination 2

Water-coordination 2 is the coordination of water across the B-X' bond of intermediate **3.7** to form the water-coordinated intermediate **3.8**. (Figure 50). In the same way, bond lengths of geometry optimized structures of **3.7** and the structures obtained from the IRC for **3.8** (reactant molecule) show different bond lengths.

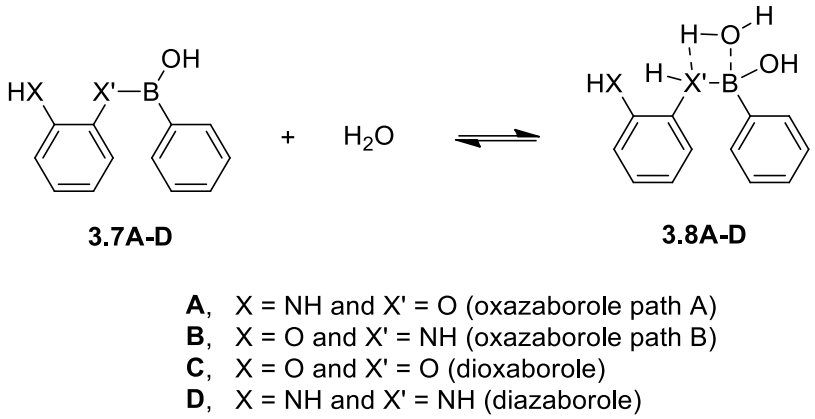


Figure 50. *Water coordination to **3.7** to give intermediate **3.8**.*

The geometry-optimized structures of **3.8** and the IRC output of **3.8** were compared similarly to the analysis in the first water coordination. In this case, the geometry around the boron of the IRC output intermediate **3.8** is approximately tetrahedral (see Figure 51). More interestingly, the geometry optimized structures of all the heteroboroles exhibited a shortening of the B-X' bond during the water coordination to the intermediate, which was the reverse of what was observed during the water coordination in the first step. A significant difference for B-X' bond was observed for **3.7A** and **3.7D** of benzodiazaborole (see Table 9).

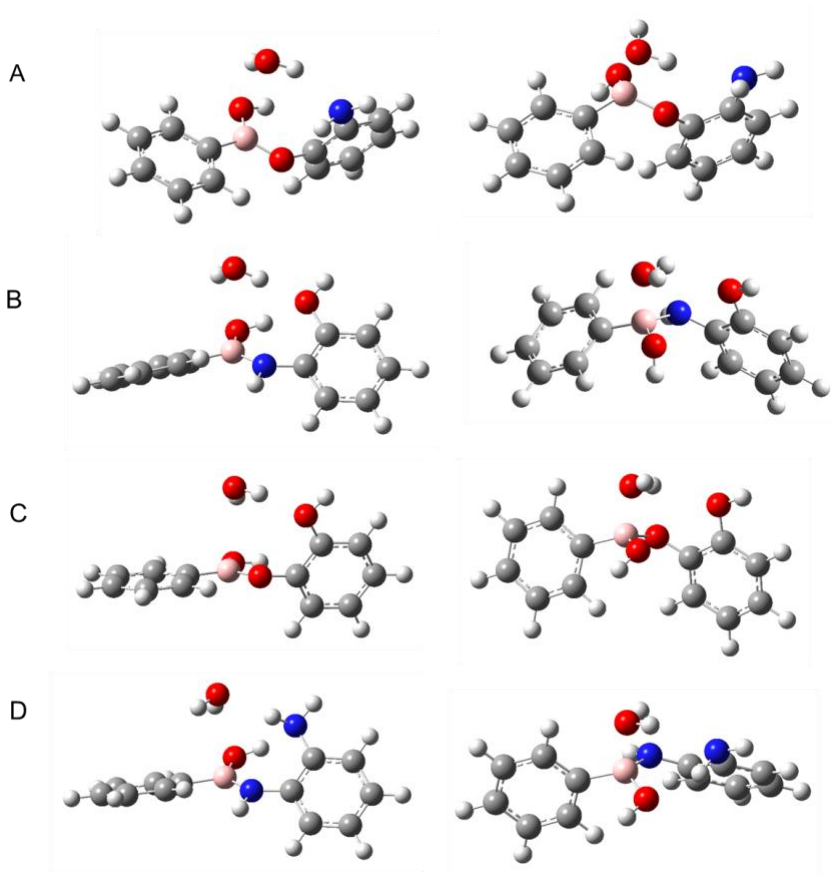


Figure 51. *Geometry-optimized (left) and IRC output (right) structures for water coordinated intermediate **3.8**.*

Table 9. *The interatomic distances (Å) of the geometry optimized structures of **3.7**, **3.8**, and IRC output structures of **3.8**.*

Heterobenzoborole	Geometry optimized structures		IRC2 output
	3.7	**3.8**	**3.8**
	B-X’	B-X’	B-X’
A	1.49	1.38	1.51
B	1.41	1.43	1.54
C	1.39	1.39	1.50
D	1.53	1.43	1.51

Conformational analysis of intermediates

When analyzing the IRC output structure of intermediates **3.7A-D**, we observed three distinct conformations, distinguished by the different orientations of the hydroxyl and amino groups. The geometry optimized structures for the intermediates resulting from a B-N bond dissociation during borole ring-opening (**3.7A** and **3.7D**) have a 5 membered ring structure with the nitrogen of the dissociated NH_2 group coordinated to the boron center similar to 3.6 in Table 6. The intermediates resulting from the O-B bond-breaking have a seven-membered ring structure (**3.7B** and **3.7C**), with a hydrogen bond between the boronic and phenolic OH groups. However, **3.7B** and **3.7C** show different orientations of intramolecular hydrogen bonding (Figure 52).

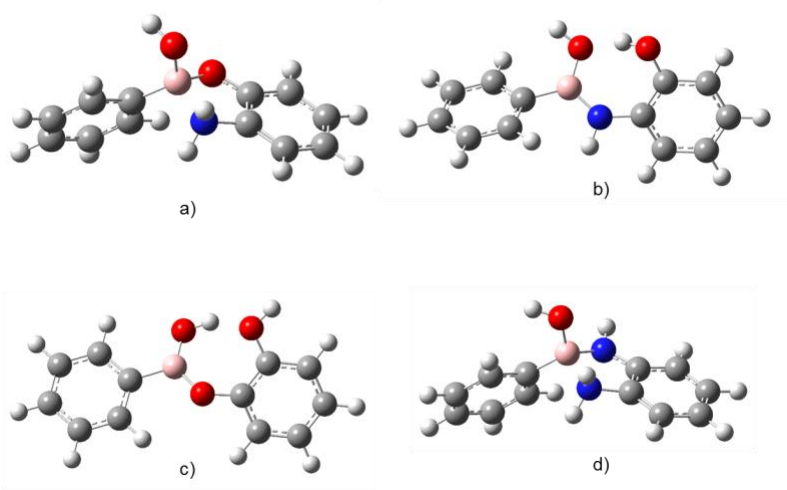


Figure 52. *Geometry-optimized structures when using structure **3.6** as the starting conformation. a) **3.7A**, b) **3.7B**, c) **3.7C**, and d) **3.7D**.*

Therefore, a thorough conformational structure analysis was carried out to study the most stable conformation. To do this we used the three distinct conformations for **3.7** as the starting point. The results of different conformations for each heterobenzoboroles using starting structures for geometry optimization with **B** and **C** are shown in Figure 53.

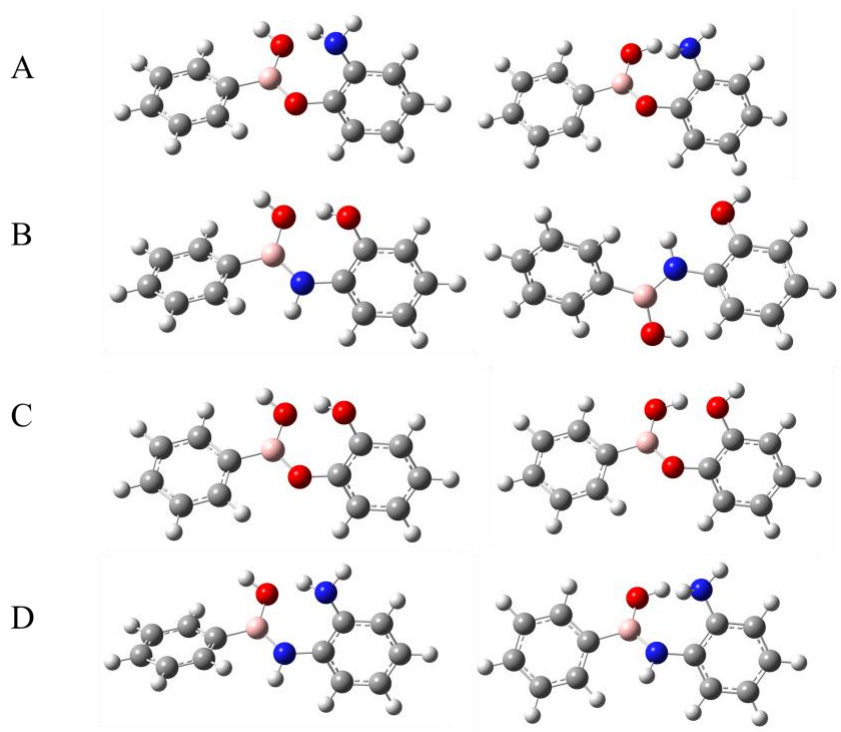


Figure 53. *Different conformations of intermediates **3.7A-D** (labeled as A-D in the figure) for each heteroborole using starting structure **B** (left) and starting structure **C** (right).*

The conformational study identified the global minima to be the seven-membered ring structure for all heterobenzoboroles (Figure 54). The lowest energy conformation for the intermediates resulting from B-N bond dissociation during borole ring-opening (**3.7A** and **3.7D**) have an intramolecular hydrogen bond H(HO)···N(NH_2), due to the nitrogen is being more basic. In the case of intermediates resulting from B-O bond dissociation (**3.7B** and **3.7C**), the intramolecular hydrogen bond H(HO)···O(B-OH) was observed as the most stable conformation. The donor and the accepter hydroxyl group pair are oriented in the opposite direction in **3.7A** or **3.7D**. This is because the hydroxyl group connected to boron (boronic acid derivate) is more basic and phenol is more acidic.

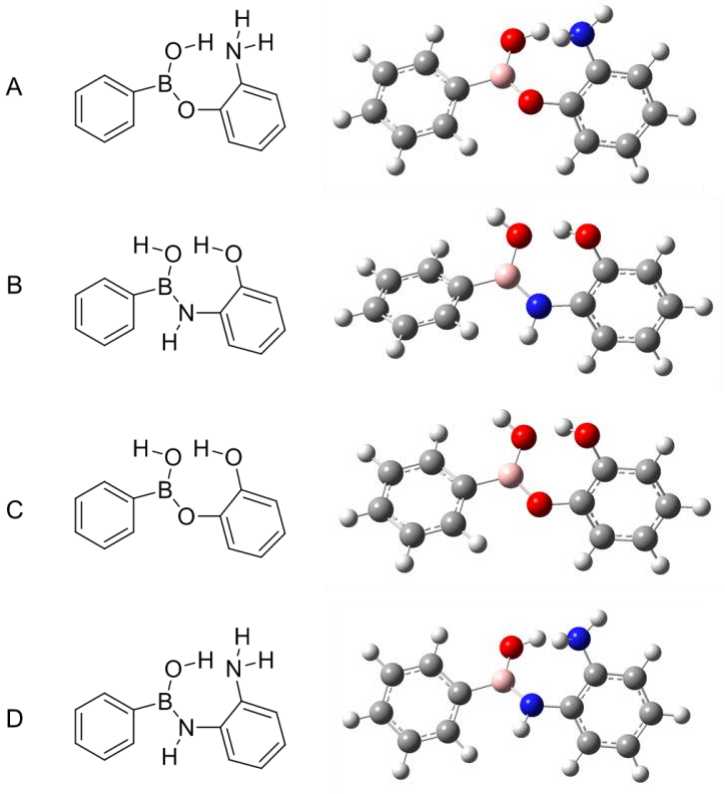


Figure 54. *Lowest energy conformations of intermediate **3.7A-D** (labeled as A-D in the figure) for each heteroborole, detailed scheme of **3.7** (left) and output structure of global minima for **3.7** (right).*

Determination of preferred pathway for hydrolysis of benzoxazaborole

Computational analysis reveals the Δ*G* of formation for **3.7A**, (**3.1A→3.7A)** is slightly exergonic by 3.11 kJ/mol. Further, the corresponding relative energy barrier (**TS1-A**) of the boron-nitrogen bond dissociation to form its corresponding intermediate **3.7A** from the unbound starting structure **3.1A** was calculated to be 109.80 kJ/mol. The energy barrier (**TS2-A**) to form the final product from the intermediate **3.7A** (**3.7A→3.2A·3.3**) was calculated to be 112.71 kJ/mol. In path B, the formation of intermediate **3.7B** from the unbound starting structure **3.1B** (**3.1B→3.7B)** is endergonic by 19.41 kJ/mol. The corresponding energy barrier (**TS1-B**) was calculated to be 139.64 kJ/mol, and the energy

barrier (**TS2-B**) to form the final product from the intermediate **3.7B** (**3.7B→3.2A·3.3**) was found to be 108.73 kJ/mol. By considering the energy barriers of both path A and B, the highest energy barrier was calculated to be 139.64 kJ/mol for **TS1-B**, (**3.1B→3.7B)**. Therefore, according to the reaction pathway for hydrolysis of benzoxazaborole **3.1**, path A is more favorable with B–N bond dissociation having a relatively lower transition state energy than that of B-O bond dissociation. Figure 55 illustrates the partial reaction coordinate for the hydrolysis of **3.1** illustrating the differences between path-A and path-B.

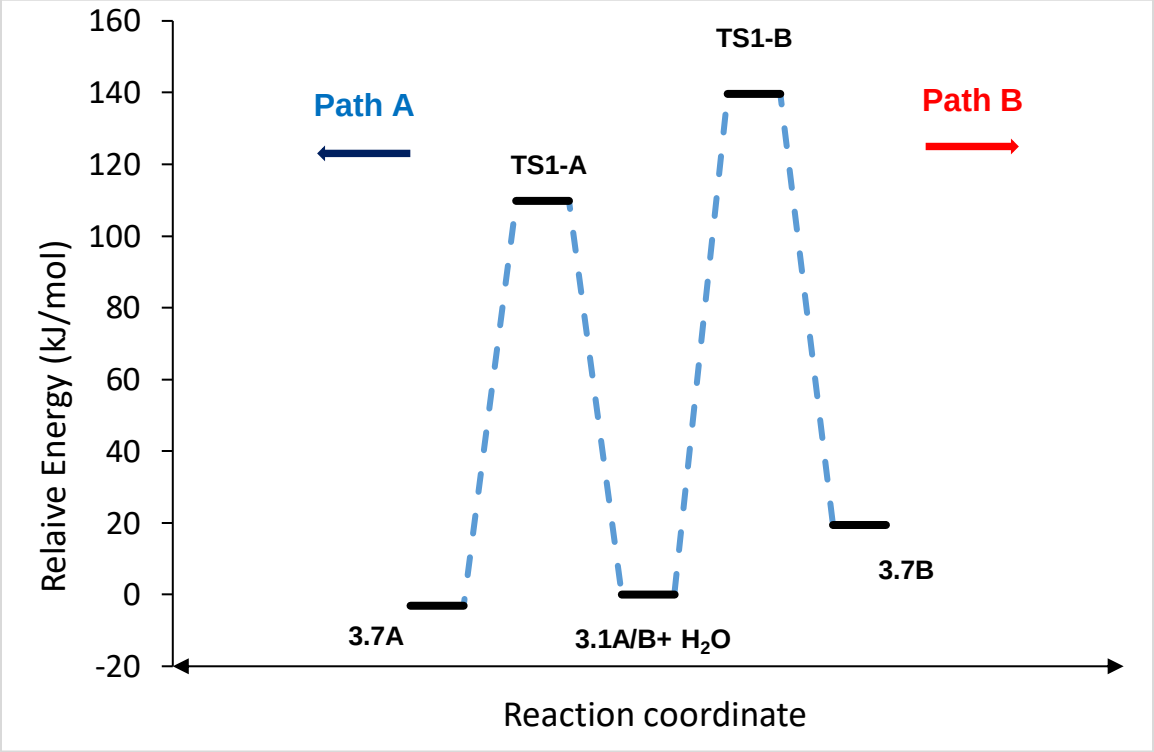


Figure 55. *Partial reaction coordinate diagram for the first step in the hydrolysis of benzoxazaborole.*

Comparison of the free energy of reactants, intermediates, and the product

The corresponding steps involved in the hydrolysis of benzoboroles are summarized in Figure 56. Step 1 is the formation of intermediate **3.7** and the energy change to form **3.7** from its unbound starting structure is defined as ΔG_1 (step 1), step 2 is the formation of products from the intermediate, and the related change in energy is denoted as ΔG_2. The overall energy difference from starting structure to form the products is defined as ΔG.

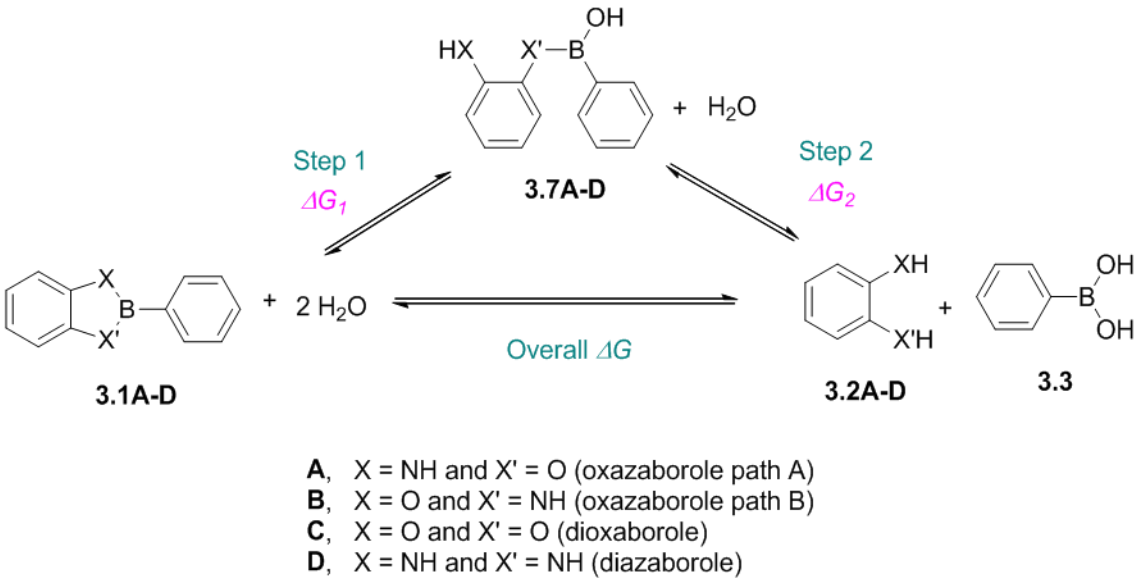


Figure 56. *Hydrolysis showing thermodynamic steps, values for ΔG (see Table 10).*

The main thermodynamic steps of hydrolysis of heteroboroles, and the relative energies were compared with the starting free heteroborole (see Table 10). The energies of the intermediates were calculated, and those formed through initial B-N bond dissociation (**3.7A** and **3.7D**) are relatively lower in energy than those formed through B-O bond dissociation. The only intermediate that was more stable than the starting heteroborole (**3.1A**) was observed in path A of benzoxazaborole hydrolysis, which is -3.11 kJ/mol more stable than the starting free heteroborole (**3.1A**), and the lifetime of **3.7A** might be higher relative to other intermediates.

In contrast, the intermediates that result from the B-O dissociation, intermediates **3.7B** and **3.7C**, are higher energy compared to the free starting structures, having 19.41 kJ/mol and 10.00 kJ/mol, respectively. Since step 1 for the hydrolysis of **3.1B** and **3.1C** are endergonic with relatively higher ΔG_1, and the formation of **3.7B** and **3.7C** is less energetically favorable (Table 10). Therefore, the hydrolysis is less favorable, and there is a higher probability of going in the reverse direction compared to the forward direction under dynamic conditions for path **B** and **C**.

Step 2 is exergonic for all heterobenzoborole systems. For path **B** and path **D** it is significantly lower compared to path **A** and **C** with -28.75 kJ/mol and -24.69 kJ/mol, respectively. Moreover, the corresponding energies for steps 1 and 2 are nearly identical with the opposite sign for the benzodioxaborole **3.1C**. Therefore, the overall Gibbs free energy (ΔG) for hydrolysis of **3.1C** was calculated to be -0.14 kJ/mol, which is relatively small compared with other heterobenzoboroles, indicating that the hydrolysis is less favorable for benzodioxaborole compared with the other heterobenzoboroles. The most notable ΔG for the overall reaction for hydrolysis was observed for path **D** (-22.44 kJ/mol) reflecting a higher likelihood to undergo hydrolysis (see Table 10).

Table 10. *The computational Gibbs free energies of step 1 and step 2 for the hydrolysis of heterobenzoborole using DFT/ω-B97XD/6-31G(d,p) in the gas phase.*

Heterobenzoborole	**Step 1** $\Delta G1$ (kJ/mol)	**Step 2** $\Delta G2$ (kJ/mol)	**Overall** ΔG (kJ/mol)
3.1A	-3.11	-6.22	-9.34
3.1B	19.41	-28.75	-9.34
3.1C	10.00	-10.15	-0.14
3.1D	2.25	-24.69	-22.44

Summary of the Transition States of heterobenzoboroles

The relative energy values for each transition state, **TS1** and **TS2**, which were calculated from both the bound and unbound starting materials, are summarized in Table 11. The **TS1** energy for the unbound state was calculated starting from the sum of free energies of the free heteroborole **3.1** and water. Similarly, the **TS1** energy for the bound complex was calculated starting from the water coordinated heteroborole (also known as complex **3.4**). Since the first water coordination is endergonic for all heteroboroles, the calculated **TS1** energy from free/unbound heteroborole is higher for every heteroborole than that calculated from the bound/water coordinated heteroborole.

Further, the **TS2** energy for the bound complex was calculated by starting from the water coordinated intermediate **3.8**. Correspondingly, the **TS2** for the unbound energy barrier was determined by starting from the sum of free energy of free intermediate **3.7** and water (see Table 11). The energy barrier 2 (**TS2**) shows a higher energy difference when calculated from bound complex than that from the unbound/ free structure for **3.1A**, and **3.1D**, which demonstrates that the second water coordination is exergonic for intermediates **3.7A** and **3.7D**, respectively. In contrast, the energy barrier is lower for the bound intermediates **3.7B** and **3.7C** compared with the energy barrier computed from the unbound starting material indicating that the second water coordination is endergonic for **3.7B** and **3.7C** (see Table 11).

Table 11. *Energy barriers 1 and 2 (**TS1** and **TS2**) calculated from the free (unbound) and bound structure at QST3/DFT/ω-B97XD/6-31G(d,p)/gas phase.*

Heterobenzoborole	**TS1** (bound)	**TS1** (unbound)	**TS2** (bound)	**TS2** (unbound)
	(kJ/mol)			
3.1A	91.46	109.80	113.80	112.71
3.1B	126.54	139.64	93.21	108.73
3.1C	109.60	116.33	91.58	104.92
3.1D	115.09	125.66	104.44	96.10

The highest activation energy can be seen for the **TS1-B**, benzoxazaborole path B hydrolysis (139.64 kJ/mol), which is significantly higher than that of its **TS2-B**; and both transition states 1 and 2 (**TS1-A** and **TS2-A**) of path A. Since the energy of **TS1-B** is significantly higher, the hydrolysis of benzoxazaborole through path B is unfavorable compared to path A. Therefore, we predict that path A is favorable for hydrolysis of benzoxazaborole.

The next highest activation barrier is seen for the benzodiazaborole **3.1D** (125.66 kJ/mol). However, transition state 2 (**TS2-D**) is significantly lower compared to the **TS1-D** transition state. Because the first transition state is greater, the kinetics of hydrolysis, the opening of the borole ring (the formation of intermediate), is slower for the diazaborole but once the intermediate is formed the conversion of product is relatively easy as the second energy barrier is lower (96.10 kJ/mol) compared to the **TS1-D**, and this observation supports the experimental data in chapter 2. In addition, energy barriers for

benzodioxaborole **3.1C** are 116.33 kJ/mol and 104.92 kJ/mol, respectively indicating that the first energy barrier is slightly higher than that of its second energy barrier.

To further study the kinetics of hydrolysis, we have chosen the unbound **TS** energies, which is the energy difference between **TS** and the sum of free energy of free structure and water. The **TS1** and **TS2** discussed above have been calculated from different starting points, for instance, **TS1** was calculated starting from the structure as **3.1**, and **TS2** was calculated starting structure as **3.7**. To compare **TS1** and **TS2** directly, we have calculated both energy barriers relative to the one single starting point, by normalizing/referencing the energy difference to the unbound structure **3.1** (see Table 12).

Table 12. *Energy barriers 1 and 2 (**TS1** and **TS2**) calculated from the free structure (unbound) **3.1**.*

Heterobenzoborole	**TS1**	**TS2**
	(kJ/mol)	
3.1A	109.80	109.60
3.1B	139.64	128.14
3.1C	116.33	114.92
3.1D	125.66	98.35

By examining Table 12, the data are more consistent, and **TS1** and **TS2** are more comparable. The computed results indicate that there is no significant difference between **TS1** and **TS2**, which have nearly identical energy barriers for hydrolysis for path A benzoxazaborole **3.1A** and benzodioxaborole **3.1C** (see Table 12). On the other hand, a substantial difference has been observed between **TS1** and **TS2** for hydrolysis through path B benzoxazaborole **3.1B** and benzodiazaborole **3.1D**, and **TS1** is higher than that of the

TS2 for both pathways indicating that the borole ring opening is kinetically unfavorable compared to the product formation.

Using the hydrolysis data in Table 12, we can gain insight into the formation of heterobenzoborole as these reactions are dynamic, and assuming reactions are microscopically reversible, meaning that the reactants and products undergo the same intermediates and same transition states in the reaction coordinate. Both path A and C have approximately similar energy barriers for both **TS1** and **TS2** denoting the rate of formation of **3.1A** and **3.1C** are fast/ favorable, which supports the experimental data in chapter 2 having a higher percent conversion during the exchange. Computed results predict that the rate of formation of **3.1B** and **3.1D** is slow with activation barriers of 139.64 kJ/mol and 125.66 kJ/mol respectively (see Table 12).

Conclusion

The hydrolytic stability of three different heterobenzoboroles has been investigated via a proposed reaction pathway analysis using density functional theory calculations (DFT) to investigate the impact on the presence of heteroatom on the five-membered borole ring. In our proposed mechanism, the hydrolysis of the boronate ester linkage undergoes a two-step reaction. In the first step, one water molecule reacts with one B–X bond and breaks the five-membered borole ring, and in the following step, another water molecule reacts with the remaining B–X' bond and generates product. These two steps have energy barriers of **TS1** and **TS2**.

Benzodioxaborole **3.1C** was found to have higher hydrolytic stability compared to other heterobenzoborole systems with having small overall Gibbs free energy difference upon hydrolysis (-0.14 kJ/mol). Moreover, this is further supported by the relative energy

of the resulting intermediate (**3.7**) upon hydrolysis of benzoxazaborole (path **A**) and benzodiazaborole **D**, which shows a relatively favorable $\Delta G_{reaction}$ (-3.44 kJ/mol and 2.25 kJ/mol), therefore, hydrolysis of **3.1A** and **3.1D** are favored. In contrast, the resulting intermediates for benzoxazaborole path B and benzodioxaborole (**3.7B** and **3.7C**) are relatively higher energy intermediates (19.41 kJ/mol and 10.00 kJ/mol respectively), indicating increased hydrolytic stability.

Based on the computed data, after normalizing each transition state to the reactant **3.1**, the ring-opening step was found to be the rate-determining step for all the heterobenzoborole systems. Moreover, the highest energy barrier (139.64 kJ/mol). for the two reaction steps was found to be for the borole ring-opening step of benzoxazaborole path B (**TS1-B**), indicating hydrolysis for benzoxazaborole is preferred through path A, B-N bond dissociation during borole ring opening.

The second highest energy barrier is seen for the benzodiazaborole **3.1D** (125.66 kJ/mol). However, transition state 2 is significantly lower compared to its first transition state, which leads to the understanding that the borole ring-opening (the formation of intermediate) is slower for the diazaborole but once the intermediate is formed the conversion of product is relatively favorable, and this observation supports the experimental data in chapter 2 as the exchange reactions involving benzodiazaborole is very slow and apparent equilibrium reached after approximately two weeks.

When we consider the reverse of hydrolysis, the formation of heterobenzoborole, and assuming reactions are dynamic and microscopically reversible, path A and C have approximately similar energy barriers for both transition states meaning the rate of

formation of **3.1A** and **3.1C** are fast/ favorable, which is in line with the experimental data in chapter 2.

Future directions

The binding energy calculations will be performed with the counterpoise correction method[39,48] to overcome the basis set superposition error (BSSE) on the complexes/ dimers. In addition, the interaction energy calculations of complexes (**3.4A**-**D** and **3.8A**-**D**) will be studied to further understanding water coordination.

To compare the stability of non(alkyl)benzoxazaborole with alkyl benzoxazaboroles, the mechanism of hydrolysis will be studied. This study will help to compare the thermodynamics and kinetics on the formation/hydrolysis of the alkyl benzoxazaborole system with the non(alkyl)benzoxazaborole, benzodioxaborole, and benzodiazaborole.

Moreover, to further support the experimental results computational chemistry will be used to study the exchange of phenyl benzoboroles, which was investigated experimentally previously by former group members[29,38] and currently in chapter II. For this, calculations will be carried out to predict the intrinsic reaction coordinates. These combined computational and experimental results will provide insight into the mechanism of heteroborole exchange, as well as optimized geometries, electronic and chemical properties of intermediates, and transition states.

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APPENDIX

CHAPTER 3 – COMPUTATIONAL OUTPUT FILES (PART OF GAUSSIAN LOG FILES)

1. Benzoxazaborole 3.1

```
%nprocshared=2
 Will use up to    2 processors via shared memory.
 %mem=1GB
 %chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\Method validatio
 n\OPT-FREQ-BOAB-CH3 basis set-GAS PHASE.chk
 ----------------------------
 # opt freq wb97xd/6-31g(d,p)
 ----------------------------
 1/14=-1,18=20,19=15,26=3,38=1/1,3;
 2/9=110,12=2,17=6,18=5,40=1/2;
 3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
 4//1;
 5/5=2,38=5/2;
 6/7=2,8=2,9=2,10=2,28=1/1;
 7//1,2,3,16;
 1/14=-1,18=20,19=15,26=3/3(2);
 2/9=110/2;
 99//99;
 2/9=110/2;
 3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
 4/5=5,16=3,69=1/1;
 5/5=2,38=5/2;
 7//1,2,3,16;
 1/14=-1,18=20,19=15,26=3/3(-5);
 2/9=110/2;
 6/7=2,8=2,9=2,10=2,19=2,28=1/1;
 99/9=1/99;
 ------------------
 Title Card Required
 ------------------
 Symbolic Z-matrix:
 Charge =  0 Multiplicity = 1
 C                 -1.84786  -0.65318  -0.00013
 C                 -1.92876   0.74756   0.00011
 C                 -3.16424   1.38374   0.00024
 C                 -4.3087    0.57957   0.00014
 C                 -4.21689  -0.81458  -0.00009
```

C	-2.97243	-1.45591	-0.00023
H	-3.24251	2.46509	0.00042
H	-5.28525	1.04966	0.00025
H	-5.12177	-1.4106	-0.00017
H	-2.88509	-2.53532	-0.00041
B	0.26465	0.09783	-0.00004
C	1.81127	0.0444	-0.00004
C	2.59597	1.21036	-0.00035
C	2.47707	-1.19366	0.00031
C	3.98651	1.14688	-0.00031
H	2.11842	2.18572	-0.00066
C	3.8676	-1.26352	0.00036
H	1.89302	-2.10727	0.00055
C	4.62552	-0.09293	0.00005
H	4.57203	2.05968	-0.00057
H	4.36146	-2.22903	0.00064
H	5.70873	-0.14578	0.00009
N	-0.61543	1.22589	0.00015
H	-0.40875	2.21055	0.00041
O	-0.53447	-1.05568	-0.00022

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.

Item	Value	Threshold	Converged?
Maximum Force	0.000167	0.000450	YES
RMS Force	0.000036	0.000300	YES
Maximum Displacement	0.001539	0.001800	YES
RMS Displacement	0.000426	0.001200	YES

Predicted change in Energy=-2.899373D-07
Optimization completed.
-- Stationary point found.

! Optimized Parameters !
! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.	
! R1	R(1,2)	1.4002	-DE/DX =	0.0001 !
! R2	R(1,6)	1.3802	-DE/DX =	0.0001 !
! R3	R(1,25)	1.3663	-DE/DX =	0.0 !
! R4	R(2,3)	1.3869	-DE/DX =	0.0 !
! R5	R(2,23)	1.3939	-DE/DX =	0.0002 !
! R6	R(3,4)	1.3967	-DE/DX =	-0.0001 !
! R7	R(3,7)	1.0852	-DE/DX =	0.0 !

```
! R8    R(4,5)            1.3946       -DE/DX =    0.0001          !
! R9    R(4,8)            1.085        -DE/DX =    0.0             !
! R10   R(5,6)            1.3973       -DE/DX =   -0.0001          !
! R11   R(5,9)            1.0849       -DE/DX =    0.0             !
! R12   R(6,10)           1.0839       -DE/DX =    0.0             !
! R13   R(11,12)          1.5522       -DE/DX =    0.0             !
! R14   R(11,23)          1.4262       -DE/DX =    0.0             !
! R15   R(11,25)          1.3972       -DE/DX =   -0.0001          !
! R16   R(12,13)          1.4015       -DE/DX =    0.0             !
! R17   R(12,14)          1.4017       -DE/DX =    0.0001          !
! R18   R(13,15)          1.3902       -DE/DX =    0.0001          !
! R19   R(13,16)          1.0875       -DE/DX =    0.0             !
! R20   R(14,17)          1.3903       -DE/DX =    0.0001          !
! R21   R(14,18)          1.0861       -DE/DX =    0.0             !
! R22   R(15,19)          1.3925       -DE/DX =    0.0             !
! R23   R(15,20)          1.0856       -DE/DX =    0.0             !
! R24   R(17,19)          1.3924       -DE/DX =    0.0             !
! R25   R(17,21)          1.0855       -DE/DX =    0.0             !
! R26   R(19,22)          1.0858       -DE/DX =    0.0             !
! R27   R(23,24)          1.0048       -DE/DX =    0.0             !
! A1    A(2,1,6)          122.2046     -DE/DX =   -0.0001          !
! A2    A(2,1,25)         110.5861     -DE/DX =    0.0             !
! A3    A(6,1,25)         127.2093     -DE/DX =    0.0             !
! A4    A(1,2,3)          120.6056     -DE/DX =    0.0001          !
! A5    A(1,2,23)         106.7433     -DE/DX =   -0.0001          !
! A6    A(3,2,23)         132.651      -DE/DX =    0.0             !
! A7    A(2,3,4)          117.6104     -DE/DX =    0.0             !
! A8    A(2,3,7)          121.3417     -DE/DX =    0.0             !
! A9    A(4,3,7)          121.0479     -DE/DX =    0.0             !
! A10   A(3,4,5)          121.3492     -DE/DX =    0.0             !
! A11   A(3,4,8)          119.1392     -DE/DX =    0.0             !
! A12   A(5,4,8)          119.5116     -DE/DX =    0.0             !
! A13   A(4,5,6)          121.0551     -DE/DX =    0.0             !
! A14   A(4,5,9)          119.5698     -DE/DX =    0.0             !
! A15   A(6,5,9)          119.375      -DE/DX =    0.0             !
! A16   A(1,6,5)          117.175      -DE/DX =    0.0             !
! A17   A(1,6,10)         120.7622     -DE/DX =    0.0             !
! A18   A(5,6,10)         122.0627     -DE/DX =    0.0             !
! A19   A(12,11,23)       129.7949     -DE/DX =    0.0             !
! A20   A(12,11,25)       122.3013     -DE/DX =   -0.0001          !
! A21   A(23,11,25)       107.9039     -DE/DX =    0.0001          !
! A22   A(11,12,13)       121.9879     -DE/DX =    0.0             !
! A23   A(11,12,14)       119.9984     -DE/DX =   -0.0001          !
! A24   A(13,12,14)       118.0137     -DE/DX =    0.0001          !
! A25   A(12,13,15)       121.2185     -DE/DX =    0.0             !
! A26   A(12,13,16)       119.9033     -DE/DX =    0.0             !
```

```
! A27   A(15,13,16)         118.8782         -DE/DX =    0.0              !
! A28   A(12,14,17)         121.0947         -DE/DX =    0.0              !
! A29   A(12,14,18)         119.1367         -DE/DX =    0.0              !
! A30   A(17,14,18)         119.7686         -DE/DX =    0.0              !
! A31   A(13,15,19)         119.8168         -DE/DX =    0.0              !
! A32   A(13,15,20)         120.0646         -DE/DX =    0.0              !
! A33   A(19,15,20)         120.1186         -DE/DX =    0.0              !
! A34   A(14,17,19)         119.9334         -DE/DX =    0.0              !
! A35   A(14,17,21)         120.0271         -DE/DX =    0.0              !
! A36   A(19,17,21)         120.0395         -DE/DX =    0.0              !
! A37   A(15,19,17)         119.9228         -DE/DX =    0.0              !
! A38   A(15,19,22)         120.0405         -DE/DX =    0.0              !
! A39   A(17,19,22)         120.0367         -DE/DX =    0.0              !
! A40   A(2,23,11)          107.4771         -DE/DX =    0.0              !
! A41   A(2,23,24)          121.9816         -DE/DX =    0.0              !
! A42   A(11,23,24)         130.5413         -DE/DX =    0.0001           !
! A43   A(1,25,11)          107.2896         -DE/DX =    0.0              !
! D1    D(6,1,2,3)            0.0006       -DE/DX =    0.0              !
! D2    D(6,1,2,23)        -179.9997         -DE/DX =    0.0              !
! D3    D(25,1,2,3)        -179.9992         -DE/DX =    0.0              !
! D4    D(25,1,2,23)          0.0005         -DE/DX =    0.0              !
! D5    D(2,1,6,5)           -0.0005       -DE/DX =    0.0              !
! D6    D(2,1,6,10)         179.9995         -DE/DX =    0.0              !
! D7    D(25,1,6,5)         179.9992         -DE/DX =    0.0              !
! D8    D(25,1,6,10)         -0.0008         -DE/DX =    0.0              !
! D9    D(2,1,25,11)          0.0001         -DE/DX =    0.0              !
! D10   D(6,1,25,11)       -179.9996          -DE/DX =    0.0              !
! D11   D(1,2,3,4)           -0.0002         -DE/DX =    0.0              !
! D12   D(1,2,3,7)          179.9993         -DE/DX =    0.0              !
! D13   D(23,2,3,4)        -179.9998          -DE/DX =    0.0              !
! D14   D(23,2,3,7)          -0.0003         -DE/DX =    0.0              !
! D15   D(1,2,23,11)         -0.0009         -DE/DX =    0.0              !
! D16   D(1,2,23,24)       -179.9939          -DE/DX =    0.0              !
! D17   D(3,2,23,11)        179.9987         -DE/DX =    0.0              !
! D18   D(3,2,23,24)          0.0058         -DE/DX =    0.0              !
! D19   D(2,3,4,5)           -0.0003         -DE/DX =    0.0              !
! D20   D(2,3,4,8)          179.9996         -DE/DX =    0.0              !
! D21   D(7,3,4,5)         -179.9997         -DE/DX =    0.0              !
! D22   D(7,3,4,8)            0.0001         -DE/DX =    0.0              !
! D23   D(3,4,5,6)            0.0003         -DE/DX =    0.0              !
! D24   D(3,4,5,9)         -179.9998         -DE/DX =    0.0              !
! D25   D(8,4,5,6)         -179.9995         -DE/DX =    0.0              !
! D26   D(8,4,5,9)            0.0003         -DE/DX =    0.0              !
! D27   D(4,5,6,1)            0.0001         -DE/DX =    0.0              !
! D28   D(4,5,6,10)        -179.9999          -DE/DX =    0.0              !
! D29   D(9,5,6,1)         -179.9998         -DE/DX =    0.0              !
```

```
 ! D30   D(9,5,6,10)          0.0003         -DE/DX =    0.0              !
 ! D31   D(23,11,12,13)       -0.0238         -DE/DX =    0.0              !
 ! D32   D(23,11,12,14)       179.9746        -DE/DX =    0.0              !
 ! D33   D(25,11,12,13)       179.9782        -DE/DX =    0.0              !
 ! D34   D(25,11,12,14)       -0.0234         -DE/DX =    0.0              !
 ! D35   D(12,11,23,2)        -179.9972       -DE/DX =    0.0              !
 ! D36   D(12,11,23,24)       -0.005          -DE/DX =    0.0              !
 ! D37   D(25,11,23,2)         0.001          -DE/DX =    0.0              !
 ! D38   D(25,11,23,24)       179.9932        -DE/DX =    0.0              !
 ! D39   D(12,11,25,1)        179.9976        -DE/DX =    0.0              !
 ! D40   D(23,11,25,1)        -0.0007         -DE/DX =    0.0              !
 ! D41   D(11,12,13,15)       179.9982        -DE/DX =    0.0              !
 ! D42   D(11,12,13,16)       -0.0036         -DE/DX =    0.0              !
 ! D43   D(14,12,13,15)       -0.0003         -DE/DX =    0.0              !
 ! D44   D(14,12,13,16)       179.9979        -DE/DX =    0.0              !
 ! D45   D(11,12,14,17)       -179.9978       -DE/DX =    0.0              !
 ! D46   D(11,12,14,18)        0.002          -DE/DX =    0.0              !
 ! D47   D(13,12,14,17)        0.0007         -DE/DX =    0.0              !
 ! D48   D(13,12,14,18)       -179.9995       -DE/DX =    0.0              !
 ! D49   D(12,13,15,19)       -0.0004         -DE/DX =    0.0              !
 ! D50   D(12,13,15,20)       179.9997        -DE/DX =    0.0              !
 ! D51   D(16,13,15,19)       -179.9987       -DE/DX =    0.0              !
 ! D52   D(16,13,15,20)        0.0014         -DE/DX =    0.0              !
 ! D53   D(12,14,17,19)       -0.0003         -DE/DX =    0.0              !
 ! D54   D(12,14,17,21)       179.9992        -DE/DX =    0.0              !
 ! D55   D(18,14,17,19)       179.9998        -DE/DX =    0.0              !
 ! D56   D(18,14,17,21)       -0.0007         -DE/DX =    0.0              !
 ! D57   D(13,15,19,17)        0.0008         -DE/DX =    0.0              !
 ! D58   D(13,15,19,22)       -179.9996       -DE/DX =    0.0              !
 ! D59   D(20,15,19,17)       -179.9993       -DE/DX =    0.0              !
 ! D60   D(20,15,19,22)        0.0003         -DE/DX =    0.0              !
 ! D61   D(14,17,19,15)       -0.0004         -DE/DX =    0.0              !
 ! D62   D(14,17,19,22)       179.9999        -DE/DX =    0.0              !
 ! D63   D(21,17,19,15)       -179.9999       -DE/DX =    0.0              !
 ! D64   D(21,17,19,22)        0.0004         -DE/DX =    0.0              !
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 - Thermochemistry -
 ------------------
Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.


 Zero-point correction=                          0.199495 (Hartree/Particle)
```

Thermal correction to Energy= 0.210557
Thermal correction to Enthalpy= 0.211501
Thermal correction to Gibbs Free Energy= 0.160158
Sum of electronic and zero-point Energies= -617.842358
Sum of electronic and thermal Energies= -617.831296
Sum of electronic and thermal Enthalpies= -617.830352
Sum of electronic and thermal Free Energies= -617.881695

2. **2-aminophenol** (**3.2A**)

---
opt wb97xd/6-31g(d,p)

1/14=-1,18=20,19=15,26=3,38=1/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4//1;
5/5=2,38=5/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(2);
2/9=110/2;
99//99;
2/9=110/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.88748	-0.75083	-0.00742
C	-0.65746	-1.40482	0.02123
C	0.53601	-0.69405	0.0189
C	0.49219	0.71637	0.00086
C	-0.7346	1.36936	0.00117
C	-1.9197	0.63807	-0.01927
H	-2.80951	-1.32087	-0.01659
H	-0.60231	-2.49023	0.03919

H	-0.77468	2.458	0.0284
H	-2.86582	1.16864	-0.03342
N	1.79965	-1.32126	0.06493
O	1.69234	1.35884	0.04962
H	2.4643	0.90795	0.39943
H	2.25513	-1.46432	0.94361
H	1.35418	-2.21244	0.15076

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Berny optimization.
Initialization pass.

Item	Value	Threshold	Converged?
Maximum Force	0.000006	0.000450	YES
RMS Force	0.000001	0.000300	YES
Maximum Displacement	0.001005	0.001800	YES
RMS Displacement	0.000227	0.001200	YES

Predicted change in Energy=-8.008809D-10
Optimization completed.
-- Stationary point found.

Optimized Parameters
(Angstroms and Degrees)

Name	Definition	Value	Derivative Info.
R1	R(1,2)	1.3919	-DE/DX = 0.0
R2	R(1,6)	1.3939	-DE/DX = 0.0
R3	R(1,7)	1.0847	-DE/DX = 0.0
R4	R(2,3)	1.3909	-DE/DX = 0.0
R5	R(2,8)	1.0871	-DE/DX = 0.0
R6	R(3,4)	1.4038	-DE/DX = 0.0
R7	R(3,11)	1.4389	-DE/DX = 0.0
R8	R(4,5)	1.3942	-DE/DX = 0.0
R9	R(4,12)	1.3469	-DE/DX = 0.0
R10	R(5,6)	1.3899	-DE/DX = 0.0
R11	R(5,9)	1.0843	-DE/DX = 0.0
R12	R(6,10)	1.0855	-DE/DX = 0.0
R13	R(11,14)	1.0141	-DE/DX = 0.0
R14	R(11,15)	1.0141	-DE/DX = 0.0
R15	R(12,13)	0.975	-DE/DX = 0.0
A1	A(2,1,6)	119.4531	-DE/DX = 0.0
A2	A(2,1,7)	120.1492	-DE/DX = 0.0
A3	A(6,1,7)	120.3977	-DE/DX = 0.0
A4	A(1,2,3)	120.4155	-DE/DX = 0.0
A5	A(1,2,8)	120.4833	-DE/DX = 0.0

```
! A6    A(3,2,8)          119.1012       -DE/DX =    0.0             !
! A7    A(2,3,4)          119.6826       -DE/DX =    0.0             !
! A8    A(2,3,11)          125.2997       -DE/DX =    0.0             !
! A9    A(4,3,11)          115.0177       -DE/DX =    0.0             !
! A10   A(3,4,5)           120.1231       -DE/DX =    0.0             !
! A11   A(3,4,12)           119.2751       -DE/DX =    0.0             !
! A12   A(5,4,12)           120.6018       -DE/DX =    0.0             !
! A13   A(4,5,6)           119.4219       -DE/DX =    0.0             !
! A14   A(4,5,9)           119.0654       -DE/DX =    0.0             !
! A15   A(6,5,9)           121.5127       -DE/DX =    0.0             !
! A16   A(1,6,5)           120.9038       -DE/DX =    0.0             !
! A17   A(1,6,10)           119.8474       -DE/DX =    0.0             !
! A18   A(5,6,10)           119.2489       -DE/DX =    0.0             !
! A19   A(3,11,14)           111.4602       -DE/DX =    0.0             !
! A20   A(3,11,15)           111.4595       -DE/DX =    0.0             !
! A21   A(14,11,15)          107.6927       -DE/DX =    0.0             !
! A22   A(4,12,13)           104.0579       -DE/DX =    0.0             !
! D1    D(6,1,2,3)          -0.0002       -DE/DX =    0.0             !
! D2    D(6,1,2,8)         -179.9993       -DE/DX =    0.0             !
! D3    D(7,1,2,3)         -180.0         -DE/DX =    0.0             !
! D4    D(7,1,2,8)           0.0008       -DE/DX =    0.0             !
! D5    D(2,1,6,5)          -0.0008       -DE/DX =    0.0             !
! D6    D(2,1,6,10)          179.9987       -DE/DX =    0.0             !
! D7    D(7,1,6,5)          179.999        -DE/DX =    0.0             !
! D8    D(7,1,6,10)          -0.0015       -DE/DX =    0.0             !
! D9    D(1,2,3,4)           0.0022       -DE/DX =    0.0             !
! D10   D(1,2,3,11)          179.9992       -DE/DX =    0.0             !
! D11   D(8,2,3,4)          180.0014       -DE/DX =    0.0             !
! D12   D(8,2,3,11)          -0.0017       -DE/DX =    0.0             !
! D13   D(2,3,4,5)           -0.0033       -DE/DX =    0.0             !
! D14   D(2,3,4,12)         -180.0031       -DE/DX =    0.0             !
! D15   D(11,3,4,5)         -180.0006       -DE/DX =    0.0             !
! D16   D(11,3,4,12)          -0.0003       -DE/DX =    0.0             !
! D17   D(2,3,11,14)         -60.1342       -DE/DX =    0.0             !
! D18   D(2,3,11,15)          60.2239       -DE/DX =    0.0             !
! D19   D(4,3,11,14)          119.8629       -DE/DX =    0.0             !
! D20   D(4,3,11,15)         -119.779        -DE/DX =    0.0             !
! D21   D(3,4,5,6)            0.0024       -DE/DX =    0.0             !
! D22   D(3,4,5,9)         -179.9987       -DE/DX =    0.0             !
! D23   D(12,4,5,6)          180.0021       -DE/DX =    0.0             !
! D24   D(12,4,5,9)            0.0011       -DE/DX =    0.0             !
! D25   D(3,4,12,13)          -0.0117       -DE/DX =    0.0             !
! D26   D(5,4,12,13)         179.9885       -DE/DX =    0.0             !
! D27   D(4,5,6,1)           -0.0003       -DE/DX =    0.0             !
! D28   D(4,5,6,10)         -179.9998       -DE/DX =    0.0             !
! D29   D(9,5,6,1)          180.0008       -DE/DX =    0.0             !
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 ! D30   D(9,5,6,10)            0.0013         -DE/DX =    0.0               !
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# freq wb97xd/6-31g(d,p)
 ----------------------
 1/10=4,30=1,38=1/1,3;
 2/12=2,17=6,18=5,40=1/2;
 3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
 4//1;
 5/5=2,38=5,98=1/2;
 8/6=4,10=90,11=11/1;
 11/6=1,8=1,9=11,15=111,16=1/1,2,10;
 10/6=1/2;
 6/7=2,8=2,9=2,10=2,18=1,28=1/1;
 7/8=1,10=1,25=1/1,2,3,16;
 1/10=4,30=1/3;
 99//99;
 -------------------
 Title Card Required
 -------------------
 Symbolic Z-matrix:
 Charge =  0 Multiplicity = 1
 C                  1.83959   0.8497    0.00001
 C                  0.57329   1.42752   0.00002
 C                 -0.56528   0.62859   0.
 C                 -0.43379  -0.769     0.00001
 C                  0.83239  -1.35268  -0.00003
 C                  1.95928  -0.53907  -0.00002
 H                  2.72458   1.47684   0.00003
 H                  0.46049   2.50878   0.00004
 H                  0.91401  -2.4339   -0.00004
 H                  2.94372  -0.99648  -0.00005
 N                 -1.9204    1.11228   0.00002
 O                 -1.54181  -1.53478   0.00005
 H                 -2.27439  -0.89136   0.00025
 H                 -2.11183   1.6796    0.81849
 H                 -2.11226   1.67846  -0.81915

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 Berny optimization.
 Initialization pass.
 Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
 Number of steps in this run=      2 maximum allowed number of steps=      2.
```

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- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.123685 (Hartree/Particle)
Thermal correction to Energy= 0.130497
Thermal correction to Enthalpy= 0.131442
Thermal correction to Gibbs Free Energy= 0.092614
Sum of electronic and zero-point Energies= -362.594234
Sum of electronic and thermal Energies= -362.587422
Sum of electronic and thermal Enthalpies= -362.586478
Sum of electronic and thermal Free Energies= -362.625305

3.Phenyl boronic acid 3.3

opt wb97xd/6-31g(d,p) geom=connectivity

1/14=-1,18=20,19=15,26=3,38=1,57=2/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4//1;
5/5=2,38=5/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(2);
2/9=110/2;
99//99;
2/9=110/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1
C -1.99012 -1.08298 0.00068
C -0.59496 -1.08298 0.00068

C	0.10258	0.12478	0.00068
C	-0.59507	1.33328	-0.00052
C	-1.9899	1.33321	-0.001
C	-2.6875	0.125	0.
H	-2.53988	-2.03529	0.00113
H	-0.04545	-2.03549	0.002
H	-2.54002	2.28549	-0.00195
H	-3.7871	0.12518	-0.00018
B	1.75258	0.1249	0.00163
O	2.52335	0.09491	-1.33126
H	3.44634	-0.10868	-1.1632
O	2.52181	0.15499	1.33542
H	3.37428	-0.27202	1.22341
H	-0.06008	2.25993	-0.00107

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Berny optimization.
Initialization pass.

Item	Value	Threshold	Converged?
Maximum Force	0.000024	0.000450	YES
RMS Force	0.000006	0.000300	YES
Maximum Displacement	0.000606	0.001800	YES
RMS Displacement	0.000147	0.001200	YES

Predicted change in Energy=-8.248114D-09
Optimization completed.
-- Stationary point found.

Optimized Parameters
(Angstroms and Degrees)

Name	Definition	Value	Derivative Info.
R1	R(1,2)	1.3909	-DE/DX = 0.0
R2	R(1,6)	1.3925	-DE/DX = 0.0
R3	R(1,7)	1.0858	-DE/DX = 0.0
R4	R(2,3)	1.401	-DE/DX = 0.0
R5	R(2,8)	1.0861	-DE/DX = 0.0
R6	R(3,4)	1.4011	-DE/DX = 0.0
R7	R(3,11)	1.5643	-DE/DX = 0.0
R8	R(4,5)	1.3909	-DE/DX = 0.0
R9	R(4,16)	1.0861	-DE/DX = 0.0
R10	R(5,6)	1.3926	-DE/DX = 0.0
R11	R(5,9)	1.0858	-DE/DX = 0.0
R12	R(6,10)	1.0861	-DE/DX = 0.0

```
! R13   R(11,12)          1.3713       -DE/DX =    0.0            !
! R14   R(11,14)          1.3713       -DE/DX =    0.0            !
! R15   R(12,13)          0.9587       -DE/DX =    0.0            !
! R16   R(14,15)          0.9587       -DE/DX =    0.0            !
! A1    A(2,1,6)         119.8703      -DE/DX =    0.0            !
! A2    A(2,1,7)         120.0699      -DE/DX =    0.0            !
! A3    A(6,1,7)         120.0598      -DE/DX =    0.0            !
! A4    A(1,2,3)         121.0906      -DE/DX =    0.0            !
! A5    A(1,2,8)         119.7372      -DE/DX =    0.0            !
! A6    A(3,2,8)         119.1723      -DE/DX =    0.0            !
! A7    A(2,3,4)         118.1357      -DE/DX =    0.0            !
! A8    A(2,3,11)         120.9258      -DE/DX =    0.0            !
! A9    A(4,3,11)         120.9386      -DE/DX =    0.0            !
! A10   A(3,4,5)          121.0904      -DE/DX =    0.0            !
! A11   A(3,4,16)          119.1695      -DE/DX =    0.0            !
! A12   A(5,4,16)          119.74       -DE/DX =    0.0            !
! A13   A(4,5,6)          119.8699      -DE/DX =    0.0            !
! A14   A(4,5,9)          120.0723      -DE/DX =    0.0            !
! A15   A(6,5,9)          120.0577      -DE/DX =    0.0            !
! A16   A(1,6,5)          119.9431      -DE/DX =    0.0            !
! A17   A(1,6,10)          120.0303      -DE/DX =    0.0            !
! A18   A(5,6,10)          120.0266      -DE/DX =    0.0            !
! A19   A(3,11,12)          118.0816      -DE/DX =    0.0            !
! A20   A(3,11,14)          118.0778      -DE/DX =    0.0            !
! A21   A(12,11,14)         123.8406      -DE/DX =    0.0            !
! A22   A(11,12,13)         115.4263      -DE/DX =    0.0            !
! A23   A(11,14,15)         115.4353      -DE/DX =    0.0            !
! D1    D(6,1,2,3)         -0.0069       -DE/DX =    0.0            !
! D2    D(6,1,2,8)         179.9902       -DE/DX =    0.0            !
! D3    D(7,1,2,3)         179.9934       -DE/DX =    0.0            !
! D4    D(7,1,2,8)         -0.0095       -DE/DX =    0.0            !
! D5    D(2,1,6,5)          0.0033       -DE/DX =    0.0            !
! D6    D(2,1,6,10)         180.006       -DE/DX =    0.0            !
! D7    D(7,1,6,5)         -179.997       -DE/DX =    0.0            !
! D8    D(7,1,6,10)         0.0056       -DE/DX =    0.0            !
! D9    D(1,2,3,4)          0.0042       -DE/DX =    0.0            !
! D10   D(1,2,3,11)        -179.9926       -DE/DX =    0.0            !
! D11   D(8,2,3,4)         -179.9929       -DE/DX =    0.0            !
! D12   D(8,2,3,11)          0.0103       -DE/DX =    0.0            !
! D13   D(2,3,4,5)           0.002       -DE/DX =    0.0            !
! D14   D(2,3,4,16)         180.0075       -DE/DX =    0.0            !
! D15   D(11,3,4,5)         179.9988       -DE/DX =    0.0            !
! D16   D(11,3,4,16)          0.0043       -DE/DX =    0.0            !
! D17   D(2,3,11,12)         -0.0155       -DE/DX =    0.0            !
! D18   D(2,3,11,14)         179.9847       -DE/DX =    0.0            !
! D19   D(4,3,11,12)        -180.0122       -DE/DX =    0.0            !
```

```
! D20   D(4,3,11,14)         -0.012         -DE/DX =    0.0              !
! D21   D(3,4,5,6)           -0.0055        -DE/DX =    0.0              !
! D22   D(3,4,5,9)           179.9955       -DE/DX =    0.0              !
! D23   D(16,4,5,6)          -180.0111      -DE/DX =    0.0              !
! D24   D(16,4,5,9)          -0.0101        -DE/DX =    0.0              !
! D25   D(4,5,6,1)           0.0028         -DE/DX =    0.0              !
! D26   D(4,5,6,10)          -179.9999      -DE/DX =    0.0              !
! D27   D(9,5,6,1)           -179.9982      -DE/DX =    0.0              !
! D28   D(9,5,6,10)          -0.0009        -DE/DX =    0.0              !
! D29   D(3,11,12,13)        179.9889       -DE/DX =    0.0              !
! D30   D(14,11,12,13)       -0.0112        -DE/DX =    0.0              !
! D31   D(3,11,14,15)        180.0105       -DE/DX =    0.0              !
! D32   D(12,11,14,15)       0.0106         -DE/DX =    0.0              !
 ---------------------------------------------------------------------------

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 ----------------------------------------
 # freq wb97xd/6-31g(d,p) geom=connectivity
 ----------------------------------------
 1/10=4,30=1,38=1,57=2/1,3;
 2/12=2,17=6,18=5,40=1/2;
 3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
 4//1;
 5/5=2,38=5,98=1/2;
 8/6=4,10=90,11=11/1;
 11/6=1,8=1,9=11,15=111,16=1/1,2,10;
 10/6=1/2;
 6/7=2,8=2,9=2,10=2,18=1,28=1/1;
 7/8=1,10=1,25=1/1,2,3,16;
 1/10=4,30=1/3;
 99//99;
 ------------------
 Title Card Required
 ------------------
 Symbolic Z-matrix:
 Charge =  0 Multiplicity = 1
 C                  1.94117   1.20567  -0.00016
 C                  0.55029   1.20174  -0.00004
 C                 -0.16981  -0.0001    0.00005
 C                  0.55044  -1.20184   0.00012
 C                  1.94133  -1.20559   0.00013
 C                  2.63812   0.0001   -0.00004
 H                  2.48256   2.14688  -0.00034
 H                  0.00891   2.14325   0.00003
 H                  2.48288  -2.1467    0.00025
```

H	3.72422	0.00014	-0.00004
B	-1.73406	-0.00002	0.00001
O	-2.37952	1.20989	0.00021
H	-3.33715	1.16552	0.00001
O	-2.37953	-1.20987	-0.00021
H	-3.33716	-1.16562	-0.00039
H	0.00915	-2.14339	0.00007

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.126729 (Hartree/Particle)
Thermal correction to Energy= 0.134583
Thermal correction to Enthalpy= 0.135527
Thermal correction to Gibbs Free Energy= 0.093906
Sum of electronic and zero-point Energies= -408.014486
Sum of electronic and thermal Energies= -408.006632
Sum of electronic and thermal Enthalpies= -408.005688
Sum of electronic and thermal Free Energies= -408.047309

4. BOAB-A-W1 3.4A

%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\TPH-01-46-OPT-BO
AB-W1-check coordination.chk
---
opt wb97xd/6-31g(d,p)

1/14=-1,18=20,19=15,26=3,38=1/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4//1;
5/5=2,38=5/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(2);
2/9=110/2;
99//99;
2/9=110/2;

3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.88086	0.75508	-0.14013
C	-1.87603	-0.62598	-0.31356
C	-3.04232	-1.35918	-0.3908
C	-4.239	-0.64226	-0.28298
C	-4.24437	0.7419	-0.10759
C	-3.05411	1.47354	-0.03321
H	-3.02572	-2.43399	-0.52856
H	-5.18181	-1.17581	-0.33709
H	-5.19152	1.26405	-0.02544
H	-3.04678	2.54832	0.10437
B	0.19911	0.07663	-0.22411
O	-0.58914	1.21166	-0.10578
C	1.74639	0.07687	-0.2557
C	2.4585	-1.11442	-0.45707
C	2.46928	1.26234	-0.06112
C	3.84942	-1.12202	-0.4668
H	1.91587	-2.04305	-0.61044
C	3.86013	1.25933	-0.07049
H	1.93501	2.19432	0.09872
C	4.55053	0.06627	-0.27336
H	4.38622	-2.05188	-0.62533
H	4.40552	2.18539	0.08058
H	5.63617	0.0625	-0.28083
O	0.21709	-0.59681	2.48335
H	1.1671	-0.4967	2.3677
H	0.02529	-1.44996	2.08214
N	-0.57872	-1.06674	-0.38862
H	-1.17725	-1.86058	-0.49629

Add virtual bond connecting atoms N27 and H26 Dist= 4.86D+00.

GradGradGradG

! R28	R(24,26)	0.9615	-DE/DX = 0.0	!
! R29	R(26,27)	2.4574	-DE/DX = 0.0	!
! R30	R(27,28)	1.0056	-DE/DX = 0.0	!
! A1	A(2,1,6)	122.1529	-DE/DX = 0.0	!
! A2	A(2,1,12)	110.6872	-DE/DX = 0.0	!
! A3	A(6,1,12)	127.1598	-DE/DX = 0.0	!
! A4	A(1,2,3)	120.7689	-DE/DX = 0.0	!
! A5	A(1,2,27)	106.7018	-DE/DX = 0.0	!
! A6	A(3,2,27)	132.5286	-DE/DX = 0.0	!
! A7	A(2,3,4)	117.5028	-DE/DX = 0.0	!
! A8	A(2,3,7)	121.3958	-DE/DX = 0.0	!
! A9	A(4,3,7)	121.1014	-DE/DX = 0.0	!
! A10	A(3,4,5)	121.3259	-DE/DX = 0.0	!
! A11	A(3,4,8)	119.1457	-DE/DX = 0.0	!
! A12	A(5,4,8)	119.528	-DE/DX = 0.0	!
! A13	A(4,5,6)	121.1351	-DE/DX = 0.0	!
! A14	A(4,5,9)	119.5164	-DE/DX = 0.0	!
! A15	A(6,5,9)	119.3484	-DE/DX = 0.0	!
! A16	A(1,6,5)	117.1131	-DE/DX = 0.0	!
! A17	A(1,6,10)	120.7688	-DE/DX = 0.0	!
! A18	A(5,6,10)	122.1179	-DE/DX = 0.0	!
! A19	A(12,11,13)	122.946	-DE/DX = 0.0	!
! A20	A(12,11,27)	108.1559	-DE/DX = 0.0	!
! A21	A(13,11,27)	128.8967	-DE/DX = 0.0	!
! A22	A(1,12,11)	107.3216	-DE/DX = 0.0	!
! A23	A(11,13,14)	121.7416	-DE/DX = 0.0	!
! A24	A(11,13,15)	120.2104	-DE/DX = 0.0	!
! A25	A(14,13,15)	118.0437	-DE/DX = 0.0	!
! A26	A(13,14,16)	121.2036	-DE/DX = 0.0	!
! A27	A(13,14,17)	119.9291	-DE/DX = 0.0	!
! A28	A(16,14,17)	118.8646	-DE/DX = 0.0	!
! A29	A(13,15,18)	121.0384	-DE/DX = 0.0	!
! A30	A(13,15,19)	119.1417	-DE/DX = 0.0	!
! A31	A(18,15,19)	119.8199	-DE/DX = 0.0	!
! A32	A(14,16,20)	119.7707	-DE/DX = 0.0	!
! A33	A(14,16,21)	120.056	-DE/DX = 0.0	!
! A34	A(20,16,21)	120.1734	-DE/DX = 0.0	!
! A35	A(15,18,20)	119.9745	-DE/DX = 0.0	!
! A36	A(15,18,22)	120.0024	-DE/DX = 0.0	!
! A37	A(20,18,22)	120.023	-DE/DX = 0.0	!
! A38	A(16,20,18)	119.9676	-DE/DX = 0.0	!
! A39	A(16,20,23)	120.0163	-DE/DX = 0.0	!
! A40	A(18,20,23)	120.0157	-DE/DX = 0.0	!
! A41	A(25,24,26)	103.7035	-DE/DX = 0.0	!
! A42	A(24,26,27)	145.5843	-DE/DX = 0.0	!
! A43	A(2,27,11)	107.1255	-DE/DX = 0.0	!

```
! A44   A(2,27,26)          103.5897       -DE/DX =    0.0             !
! A45   A(2,27,28)          121.7618       -DE/DX =    0.0             !
! A46   A(11,27,26)          79.7408       -DE/DX =    0.0             !
! A47   A(26,27,28)          94.8434       -DE/DX =    0.0             !
! A48   L(11,27,28,2,-1)     228.8873       -DE/DX =    0.0             !
! A49   L(11,27,28,2,-2)     172.1478       -DE/DX =    0.0             !
! D1    D(6,1,2,3)            0.3826       -DE/DX =    0.0             !
! D2    D(6,1,2,27)        -179.3584       -DE/DX =    0.0             !
! D3    D(12,1,2,3)        -179.5143       -DE/DX =    0.0             !
! D4    D(12,1,2,27)          0.7447       -DE/DX =    0.0             !
! D5    D(2,1,6,5)           -0.2583       -DE/DX =    0.0             !
! D6    D(2,1,6,10)         179.6091       -DE/DX =    0.0             !
! D7    D(12,1,6,5)         179.6207       -DE/DX =    0.0             !
! D8    D(12,1,6,10)         -0.5119       -DE/DX =    0.0             !
! D9    D(2,1,12,11)         -0.2604       -DE/DX =    0.0             !
! D10   D(6,1,12,11)        179.8491       -DE/DX =    0.0             !
! D11   D(1,2,3,4)           -0.1917       -DE/DX =    0.0             !
! D12   D(1,2,3,7)          179.8042       -DE/DX =    0.0             !
! D13   D(27,2,3,4)         179.4718       -DE/DX =    0.0             !
! D14   D(27,2,3,7)          -0.5324       -DE/DX =    0.0             !
! D15   D(1,2,27,11)         -0.9107       -DE/DX =    0.0             !
! D16   D(1,2,27,26)         82.3561       -DE/DX =    0.0             !
! D17   D(1,2,27,28)       -173.0585       -DE/DX =    0.0             !
! D18   D(3,2,27,11)        179.3913       -DE/DX =    0.0             !
! D19   D(3,2,27,26)         -97.342       -DE/DX =    0.0             !
! D20   D(3,2,27,28)           7.2434      -DE/DX =    0.0             !
! D21   D(2,3,4,5)            -0.1001       -DE/DX =    0.0             !
! D22   D(2,3,4,8)          -179.8843       -DE/DX =    0.0             !
! D23   D(7,3,4,5)          179.9041       -DE/DX =    0.0             !
! D24   D(7,3,4,8)            0.1198       -DE/DX =    0.0             !
! D25   D(3,4,5,6)            0.2192       -DE/DX =    0.0             !
! D26   D(3,4,5,9)         -179.7635       -DE/DX =    0.0             !
! D27   D(8,4,5,6)         -179.9974       -DE/DX =    0.0             !
! D28   D(8,4,5,9)            0.02         -DE/DX =    0.0             !
! D29   D(4,5,6,1)            -0.038        -DE/DX =    0.0             !
! D30   D(4,5,6,10)         -179.9035       -DE/DX =    0.0             !
! D31   D(9,5,6,1)          179.9446       -DE/DX =    0.0             !
! D32   D(9,5,6,10)           0.0792       -DE/DX =    0.0             !
! D33   D(13,11,12,1)      -179.9274       -DE/DX =    0.0             !
! D34   D(27,11,12,1)        -0.3205       -DE/DX =    0.0             !
! D35   D(12,11,13,14)      172.159        -DE/DX =    0.0             !
! D36   D(12,11,13,15)       -7.0631       -DE/DX =    0.0             !
! D37   D(27,11,13,14)       -7.361        -DE/DX =    0.0             !
! D38   D(27,11,13,15)      173.4169       -DE/DX =    0.0             !
! D39   D(12,11,27,2)         0.7746       -DE/DX =    0.0             !
! D40   D(12,11,27,26)     -100.4173       -DE/DX =    0.0             !
```

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 ! D41   D(13,11,27,2)       -179.6493       -DE/DX =    0.0             !
 ! D42   D(13,11,27,26)       79.1589       -DE/DX =    0.0             !
 ! D43   D(11,13,14,16)      -179.3822       -DE/DX =    0.0             !
 ! D44   D(11,13,14,17)        0.0136       -DE/DX =    0.0             !
 ! D45   D(15,13,14,16)       -0.1438       -DE/DX =    0.0             !
 ! D46   D(15,13,14,17)      179.252        -DE/DX =    0.0             !
 ! D47   D(11,13,15,18)      179.6627       -DE/DX =    0.0             !
 ! D48   D(11,13,15,19)       -0.2452       -DE/DX =    0.0             !
 ! D49   D(14,13,15,18)        0.4123       -DE/DX =    0.0             !
 ! D50   D(14,13,15,19)     -179.4957       -DE/DX =    0.0             !
 ! D51   D(13,14,16,20)       -0.2121       -DE/DX =    0.0             !
 ! D52   D(13,14,16,21)      179.7886       -DE/DX =    0.0             !
 ! D53   D(17,14,16,20)     -179.6142       -DE/DX =    0.0             !
 ! D54   D(17,14,16,21)        0.3865       -DE/DX =    0.0             !
 ! D55   D(13,15,18,20)       -0.3239       -DE/DX =    0.0             !
 ! D56   D(13,15,18,22)      179.8112       -DE/DX =    0.0             !
 ! D57   D(19,15,18,20)      179.5835       -DE/DX =    0.0             !
 ! D58   D(19,15,18,22)       -0.2814       -DE/DX =    0.0             !
 ! D59   D(14,16,20,18)        0.3066       -DE/DX =    0.0             !
 ! D60   D(14,16,20,23)     -179.9137       -DE/DX =    0.0             !
 ! D61   D(21,16,20,18)     -179.6941       -DE/DX =    0.0             !
 ! D62   D(21,16,20,23)        0.0856       -DE/DX =    0.0             !
 ! D63   D(15,18,20,16)       -0.0423       -DE/DX =    0.0             !
 ! D64   D(15,18,20,23)     -179.8219       -DE/DX =    0.0             !
 ! D65   D(22,18,20,16)      179.8226       -DE/DX =    0.0             !
 ! D66   D(22,18,20,23)        0.0429       -DE/DX =    0.0             !
 ! D67   D(25,24,26,27)      -43.1789       -DE/DX =    0.0             !
 ! D68   D(24,26,27,2)      -106.8681       -DE/DX =    0.0             !
 ! D69   D(24,26,27,11)       -1.5537       -DE/DX =    0.0             !
 ! D70   D(24,26,27,28)      128.8007       -DE/DX =    0.0             !
 --------------------------------------------------------------------------------
 GradGradGradGradGradGradGradGradGradGradGrad

**********************************************
 %nprocshared=3
 Will use up to    3 processors via shared memory.
 %mem=1GB
 %chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\TPH-01-46-
FREQ-BOAB-W1-CHECK COORDINATION.chk
 ----------------------
 # freq wb97xd/6-31g(d,p)
 ----------------------
 1/10=4,30=1,38=1/1,3;
 2/12=2,17=6,18=5,40=1/2;
 3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
 4//1;
```

5/5=2,38=5,98=1/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1/2;
6/7=2,8=2,9=2,10=2,18=1,28=1/1;
7/8=1,10=1,25=1/1,2,3,16;
1/10=4,30=1/3;
99//99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.90075	0.73839	0.05171
C	-1.97571	-0.55991	-0.46458
C	-3.20304	-1.16527	-0.68613
C	-4.3495	-0.43287	-0.37129
C	-4.2649	0.85866	0.14869
C	-3.02799	1.46876	0.36937
H	-3.27307	-2.17039	-1.08905
H	-5.32394	-0.88163	-0.53231
H	-5.17449	1.39965	0.3865
H	-2.94369	2.47054	0.77397
B	0.1988	0.07936	-0.25776
O	-0.59791	1.13401	0.17676
C	1.74979	0.1416	-0.2682
C	2.53169	-0.98672	-0.55647
C	2.40963	1.34186	0.03074
C	3.92095	-0.92136	-0.55027
H	2.05167	-1.93683	-0.78063
C	3.79781	1.41528	0.03322
H	1.82182	2.22434	0.26469
C	4.55504	0.28315	-0.25789
H	4.50781	-1.80687	-0.77273
H	4.29121	2.354	0.26409
H	5.63916	0.33902	-0.25331
O	0.54984	-1.58388	2.35623
H	1.38668	-1.28298	1.99061
H	0.01596	-1.77158	1.57886
N	-0.65957	-0.9944	-0.65243
H	-0.44965	-1.86372	-1.11229

GradGradGradG

Berny optimization.
Initialization pass.

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.223910 (Hartree/Particle)
Thermal correction to Energy= 0.238617
Thermal correction to Enthalpy= 0.239562
Thermal correction to Gibbs Free Energy= 0.180153
Sum of electronic and zero-point Energies= -694.224635
Sum of electronic and thermal Energies= -694.209927
Sum of electronic and thermal Enthalpies= -694.208983
Sum of electronic and thermal Free Energies= -694.268392

5. BOAB-INT-A-W1 3.8A

%nprocshared=3
Will use up to 3 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thusini\Reproducing data of li et. al paper\BDAB-product form
ation\TPH-01-46-OPT-BOAB-INT-1-W1-N-B break 1st-GAS PHASE-8-18.chk
---
opt wb97xd/6-31g(d,p) geom=connectivity

1/14=-1,18=20,19=15,26=3,38=1,57=2/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4//1;
5/5=2,38=5/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(2);
2/9=110/2;
99//99;
2/9=110/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.64355	-0.39405	-0.33219
C	-2.68138	0.52607	-0.13194
C	-3.94558	0.09583	0.24599
C	-4.18539	-1.26514	0.42696
C	-3.15871	-2.18323	0.24403
C	-1.89083	-1.74553	-0.13354
H	-4.74038	0.82087	0.40536
H	-5.17472	-1.59984	0.71968
H	-3.3406	-3.24205	0.39151
H	-1.07425	-2.44187	-0.2912
C	1.97644	0.07102	0.10106
C	2.86766	0.3246	1.15052
C	2.43205	-0.70196	-0.97364
C	4.16729	-0.17097	1.13017
H	2.5297	0.92266	1.99209
C	3.73122	-1.19872	-1.00451
H	1.75093	-0.92318	-1.79064
C	4.60245	-0.93261	0.0487
H	4.84412	0.03909	1.95289
H	4.0666	-1.79298	-1.84918
H	5.61548	-1.3239	0.02966
B	0.49456	0.61661	0.14804
O	0.04977	1.18766	1.32504
H	-0.85759	1.49695	1.24946
O	0.63591	2.28264	-1.027
H	-0.15234	2.00865	-1.51551
H	0.35	3.03678	-0.49955
N	-2.32559	1.94452	-0.28137
H	-2.60673	2.26519	-1.18587
H	-2.79164	2.48098	0.4222
O	-0.43526	0.04513	-0.77581

Add virtual bond connecting atoms O25 and B22 Dist= 3.86D+00.
Add virtual bond connecting atoms H26 and O31 Dist= 4.00D+00.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad GradGradGrad
Berny optimization.
Initialization pass.

Item	Value	Threshold	Converged?
Maximum Force	0.000023	0.000450	YES
RMS Force	0.000005	0.000300	YES

Maximum Displacement 0.001391 0.001800 YES
RMS Displacement 0.000464 0.001200 YES
Predicted change in Energy=-1.819637D-08
Optimization completed.
-- Stationary point found.

Optimized Parameters
(Angstroms and Degrees)

Name	Definition	Value	Derivative Info.
R1	R(1,2)	1.4039	-DE/DX = 0.0
R2	R(1,6)	1.3888	-DE/DX = 0.0
R3	R(1,31)	1.3742	-DE/DX = 0.0
R4	R(2,3)	1.3956	-DE/DX = 0.0
R5	R(2,28)	1.398	-DE/DX = 0.0
R6	R(3,4)	1.3916	-DE/DX = 0.0
R7	R(3,7)	1.0863	-DE/DX = 0.0
R8	R(4,5)	1.3904	-DE/DX = 0.0
R9	R(4,8)	1.0849	-DE/DX = 0.0
R10	R(5,6)	1.3934	-DE/DX = 0.0
R11	R(5,9)	1.0842	-DE/DX = 0.0
R12	R(6,10)	1.0854	-DE/DX = 0.0
R13	R(11,12)	1.4005	-DE/DX = 0.0
R14	R(11,13)	1.4004	-DE/DX = 0.0
R15	R(11,22)	1.5556	-DE/DX = 0.0
R16	R(12,14)	1.3902	-DE/DX = 0.0
R17	R(12,15)	1.0861	-DE/DX = 0.0
R18	R(13,16)	1.3903	-DE/DX = 0.0
R19	R(13,17)	1.0863	-DE/DX = 0.0
R20	R(14,18)	1.3928	-DE/DX = 0.0
R21	R(14,19)	1.0856	-DE/DX = 0.0
R22	R(16,18)	1.3924	-DE/DX = 0.0
R23	R(16,20)	1.0857	-DE/DX = 0.0
R24	R(18,21)	1.0859	-DE/DX = 0.0
R25	R(22,23)	1.3683	-DE/DX = 0.0
R26	R(22,25)	2.9965	-DE/DX = 0.0
R27	R(22,31)	1.3872	-DE/DX = 0.0
R28	R(23,24)	0.9636	-DE/DX = 0.0
R29	R(25,26)	0.9681	-DE/DX = 0.0
R30	R(25,27)	0.9617	-DE/DX = 0.0
R31	R(26,31)	3.1847	-DE/DX = 0.0
R32	R(28,29)	1.0128	-DE/DX = 0.0
R33	R(28,30)	1.0101	-DE/DX = 0.0
A1	A(2,1,6)	120.9962	-DE/DX = 0.0
A2	A(2,1,31)	117.7047	-DE/DX = 0.0

```
! A3    A(6,1,31)          121.2836        -DE/DX =    0.0             !
! A4    A(1,2,3)           118.3534        -DE/DX =    0.0             !
! A5    A(1,2,28)          118.8878        -DE/DX =    0.0             !
! A6    A(3,2,28)          122.674         -DE/DX =    0.0             !
! A7    A(2,3,4)           120.6438        -DE/DX =    0.0             !
! A8    A(2,3,7)           119.1392        -DE/DX =    0.0             !
! A9    A(4,3,7)           120.2152        -DE/DX =    0.0             !
! A10   A(3,4,5)           120.5378        -DE/DX =    0.0             !
! A11   A(3,4,8)           119.343         -DE/DX =    0.0             !
! A12   A(5,4,8)           120.1191        -DE/DX =    0.0             !
! A13   A(4,5,6)           119.4257        -DE/DX =    0.0             !
! A14   A(4,5,9)           120.6262        -DE/DX =    0.0             !
! A15   A(6,5,9)           119.9475        -DE/DX =    0.0             !
! A16   A(1,6,5)           120.0421        -DE/DX =    0.0             !
! A17   A(1,6,10)          118.6371        -DE/DX =    0.0             !
! A18   A(5,6,10)          121.3164        -DE/DX =    0.0             !
! A19   A(12,11,13)        118.2727        -DE/DX =    0.0             !
! A20   A(12,11,22)        120.7932        -DE/DX =    0.0             !
! A21   A(13,11,22)        120.9339        -DE/DX =    0.0             !
! A22   A(11,12,14)        121.0064        -DE/DX =    0.0             !
! A23   A(11,12,15)        119.2294        -DE/DX =    0.0             !
! A24   A(14,12,15)        119.764         -DE/DX =    0.0             !
! A25   A(11,13,16)        121.04          -DE/DX =    0.0             !
! A26   A(11,13,17)        119.2051        -DE/DX =    0.0             !
! A27   A(16,13,17)        119.7549        -DE/DX =    0.0             !
! A28   A(12,14,18)        119.8561        -DE/DX =    0.0             !
! A29   A(12,14,19)        120.1389        -DE/DX =    0.0             !
! A30   A(18,14,19)        120.005         -DE/DX =    0.0             !
! A31   A(13,16,18)        119.826         -DE/DX =    0.0             !
! A32   A(13,16,20)        120.1171        -DE/DX =    0.0             !
! A33   A(18,16,20)        120.057         -DE/DX =    0.0             !
! A34   A(14,18,16)        119.9987        -DE/DX =    0.0             !
! A35   A(14,18,21)        119.9562        -DE/DX =    0.0             !
! A36   A(16,18,21)        120.0451        -DE/DX =    0.0             !
! A37   A(11,22,23)        120.4058        -DE/DX =    0.0             !
! A38   A(11,22,25)         95.2971        -DE/DX =    0.0             !
! A39   A(11,22,31)        118.141         -DE/DX =    0.0             !
! A40   A(23,22,25)         77.4912        -DE/DX =    0.0             !
! A41   A(23,22,31)        121.4155        -DE/DX =    0.0             !
! A42   A(25,22,31)         99.3845        -DE/DX =    0.0             !
! A43   A(22,23,24)        112.7066        -DE/DX =    0.0             !
! A44   A(22,25,26)         84.0368        -DE/DX =    0.0             !
! A45   A(22,25,27)         55.838         -DE/DX =    0.0             !
! A46   A(26,25,27)        104.4712        -DE/DX =    0.0             !
! A47   A(25,26,31)        101.0229        -DE/DX =    0.0             !
! A48   A(2,28,29)         113.0425        -DE/DX =    0.0             !
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! A49	A(2,28,30)	114.3506	-DE/DX = 0.0	!
! A50	A(29,28,30)	111.8516	-DE/DX = 0.0	!
! A51	A(1,31,22)	120.8872	-DE/DX = 0.0	!
! A52	A(1,31,26)	84.7214	-DE/DX = 0.0	!
! A53	A(22,31,26)	71.843	-DE/DX = 0.0	!
! D1	D(6,1,2,3)	0.0086	-DE/DX = 0.0	!
! D2	D(6,1,2,28)	176.7506	-DE/DX = 0.0	!
! D3	D(31,1,2,3)	178.59	-DE/DX = 0.0	!
! D4	D(31,1,2,28)	-4.6681	-DE/DX = 0.0	!
! D5	D(2,1,6,5)	-0.2769	-DE/DX = 0.0	!
! D6	D(2,1,6,10)	178.9777	-DE/DX = 0.0	!
! D7	D(31,1,6,5)	-178.8072	-DE/DX = 0.0	!
! D8	D(31,1,6,10)	0.4474	-DE/DX = 0.0	!
! D9	D(2,1,31,22)	102.4631	-DE/DX = 0.0	!
! D10	D(2,1,31,26)	37.2934	-DE/DX = 0.0	!
! D11	D(6,1,31,22)	-78.9598	-DE/DX = 0.0	!
! D12	D(6,1,31,26)	-144.1295	-DE/DX = 0.0	!
! D13	D(1,2,3,4)	0.2117	-DE/DX = 0.0	!
! D14	D(1,2,3,7)	179.7187	-DE/DX = 0.0	!
! D15	D(28,2,3,4)	-176.3993	-DE/DX = 0.0	!
! D16	D(28,2,3,7)	3.1078	-DE/DX = 0.0	!
! D17	D(1,2,28,29)	28.1382	-DE/DX = 0.0	!
! D18	D(1,2,28,30)	157.6678	-DE/DX = 0.0	!
! D19	D(3,2,28,29)	-155.2682	-DE/DX = 0.0	!
! D20	D(3,2,28,30)	-25.7385	-DE/DX = 0.0	!
! D21	D(2,3,4,5)	-0.1653	-DE/DX = 0.0	!
! D22	D(2,3,4,8)	179.9291	-DE/DX = 0.0	!
! D23	D(7,3,4,5)	-179.6671	-DE/DX = 0.0	!
! D24	D(7,3,4,8)	0.4274	-DE/DX = 0.0	!
! D25	D(3,4,5,6)	-0.1048	-DE/DX = 0.0	!
! D26	D(3,4,5,9)	-179.8196	-DE/DX = 0.0	!
! D27	D(8,4,5,6)	179.8	-DE/DX = 0.0	!
! D28	D(8,4,5,9)	0.0852	-DE/DX = 0.0	!
! D29	D(4,5,6,1)	0.3232	-DE/DX = 0.0	!
! D30	D(4,5,6,10)	-178.911	-DE/DX = 0.0	!
! D31	D(9,5,6,1)	-179.96	-DE/DX = 0.0	!
! D32	D(9,5,6,10)	0.8058	-DE/DX = 0.0	!
! D33	D(13,11,12,14)	0.1444	-DE/DX = 0.0	!
! D34	D(13,11,12,15)	179.9931	-DE/DX = 0.0	!
! D35	D(22,11,12,14)	179.9679	-DE/DX = 0.0	!
! D36	D(22,11,12,15)	-0.1833	-DE/DX = 0.0	!
! D37	D(12,11,13,16)	-0.0548	-DE/DX = 0.0	!
! D38	D(12,11,13,17)	179.8446	-DE/DX = 0.0	!
! D39	D(22,11,13,16)	-179.878	-DE/DX = 0.0	!
! D40	D(22,11,13,17)	0.0213	-DE/DX = 0.0	!
! D41	D(12,11,22,23)	-2.9964	-DE/DX = 0.0	!

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 ! D42   D(12,11,22,25)      75.5954      -DE/DX =    0.0            !
 ! D43   D(12,11,22,31)     179.2049      -DE/DX =    0.0            !
 ! D44   D(13,11,22,23)     176.8224      -DE/DX =    0.0            !
 ! D45   D(13,11,22,25)    -104.5858      -DE/DX =    0.0            !
 ! D46   D(13,11,22,31)      -0.9763      -DE/DX =    0.0            !
 ! D47   D(11,12,14,18)      -0.1103      -DE/DX =    0.0            !
 ! D48   D(11,12,14,19)     179.8294      -DE/DX =    0.0            !
 ! D49   D(15,12,14,18)    -179.9583      -DE/DX =    0.0            !
 ! D50   D(15,12,14,19)      -0.0186      -DE/DX =    0.0            !
 ! D51   D(11,13,16,18)      -0.0683      -DE/DX =    0.0            !
 ! D52   D(11,13,16,20)     179.9377      -DE/DX =    0.0            !
 ! D53   D(17,13,16,18)    -179.9671      -DE/DX =    0.0            !
 ! D54   D(17,13,16,20)       0.0389      -DE/DX =    0.0            !
 ! D55   D(12,14,18,16)      -0.016       -DE/DX =    0.0            !
 ! D56   D(12,14,18,21)     179.9831      -DE/DX =    0.0            !
 ! D57   D(19,14,18,16)    -179.9559      -DE/DX =    0.0            !
 ! D58   D(19,14,18,21)       0.0432      -DE/DX =    0.0            !
 ! D59   D(13,16,18,14)       0.1043      -DE/DX =    0.0            !
 ! D60   D(13,16,18,21)    -179.8948      -DE/DX =    0.0            !
 ! D61   D(20,16,18,14)    -179.9017      -DE/DX =    0.0            !
 ! D62   D(20,16,18,21)       0.0992      -DE/DX =    0.0            !
 ! D63   D(11,22,23,24)    -175.7418      -DE/DX =    0.0            !
 ! D64   D(25,22,23,24)      95.4355      -DE/DX =    0.0            !
 ! D65   D(31,22,23,24)       1.9836      -DE/DX =    0.0            !
 ! D66   D(11,22,25,26)     143.8304      -DE/DX =    0.0            !
 ! D67   D(11,22,25,27)    -104.1741      -DE/DX =    0.0            !
 ! D68   D(23,22,25,26)     -96.1642      -DE/DX =    0.0            !
 ! D69   D(23,22,25,27)      15.8313      -DE/DX =    0.0            !
 ! D70   D(31,22,25,26)      24.1333      -DE/DX =    0.0            !
 ! D71   D(31,22,25,27)     136.1288      -DE/DX =    0.0            !
 ! D72   D(11,22,31,1)      179.3073      -DE/DX =    0.0            !
 ! D73   D(11,22,31,26)    -108.6913      -DE/DX =    0.0            !
 ! D74   D(23,22,31,1)       1.5319      -DE/DX =    0.0            !
 ! D75   D(23,22,31,26)     73.5333      -DE/DX =    0.0            !
 ! D76   D(25,22,31,1)      -79.4763      -DE/DX =    0.0            !
 ! D77   D(25,22,31,26)      -7.4749      -DE/DX =    0.0            !
 ! D78   D(22,25,26,31)     -10.3119      -DE/DX =    0.0            !
 ! D79   D(27,25,26,31)     -62.719       -DE/DX =    0.0            !
 ! D80   D(25,26,31,1)      148.8242      -DE/DX =    0.0            !
 ! D81   D(25,26,31,22)      23.8749      -DE/DX =    0.0            !
 ---------------------------------------------------------------------------
 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 ------------------
 - Thermochemistry -
 ------------------
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
```

Zero-point correction= 0.251245 (Hartree/Particle)
Thermal correction to Energy= 0.267732
Thermal correction to Enthalpy= 0.268677
Thermal correction to Gibbs Free Energy= 0.205865
Sum of electronic and zero-point Energies= -770.625278
Sum of electronic and thermal Energies= -770.608790
Sum of electronic and thermal Enthalpies= -770.607846
Sum of electronic and thermal Free Energies= -770.670657

BOAB-TS1 (TS1-A)

%nprocshared=2
Will use up to 2 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\BOAB new\OPT-QST
3-TS1-BOAB-N-B-3-29-mirror image-trial 3-ca-with ini TSA.chk
---
opt=(calcall,qst3) wb97xd/6-31g(d,p)

1/5=1,10=4,14=-1,18=20,26=3,27=203,38=1/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
4//1;
5/5=2,38=5/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1/2;
6/7=2,8=2,9=2,10=2,18=1,28=1/1;
7/10=1,25=1/1,2,3,16;
1/5=1,10=4,14=-1,18=20,26=3,27=203/3(3);
2/9=110/2;
7/8=1,9=1,25=1,44=-1/16;
99//99;
2/9=110/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1/2;
7/10=1,25=1/1,2,3,16;
1/5=1,10=4,14=-1,18=20,26=3,27=203/3(-8);
2/9=110/2;
6/7=2,8=2,9=2,10=2,18=1,19=2,28=1/1;

```
7/8=1,9=1,25=1,44=-1/16;
99//99;
------------------
Title Card Required
------------------
Symbolic Z-matrix:
Charge =  0 Multiplicity = 1
C                 -1.90075   0.73839  -0.05171
C                 -1.97571  -0.55991   0.46458
C                 -3.20304  -1.16527   0.68613
C                 -4.3495   -0.43287   0.37129
C                 -4.2649    0.85866  -0.14869
C                 -3.02799   1.46876  -0.36937
H                 -3.27307  -2.17039   1.08905
H                 -5.32394  -0.88163   0.53231
H                 -5.17449   1.39965  -0.3865
H                 -2.94369   2.47054  -0.77397
B                  0.1988    0.07936   0.25776
O                 -0.59791   1.13401  -0.17676
C                  1.74979   0.1416    0.2682
C                  2.53169  -0.98672   0.55647
C                  2.40963   1.34186  -0.03074
C                  3.92095  -0.92136   0.55027
H                  2.05167  -1.93683   0.78063
C                  3.79781   1.41528  -0.03322
H                  1.82182   2.22434  -0.26469
C                  4.55504   0.28315   0.25789
H                  4.50781  -1.80687   0.77273
H                  4.29121   2.354    -0.26409
H                  5.63916   0.33902   0.25331
O                  0.54984  -1.58388  -2.35623
H                  1.38668  -1.28298  -1.99061
H                  0.01596  -1.77158  -1.57886
N                 -0.65957  -0.9944    0.65243
H                 -0.44965  -1.86372   1.11229

Add virtual bond connecting atoms B11        and H26        Dist= 4.94D+00.
Add virtual bond connecting atoms N27        and H26        Dist= 4.64D+00.
------------------
Title Card Required
------------------
Symbolic Z-matrix:
Charge =  0 Multiplicity = 1
C                  1.75607  -0.27235  -0.60643
C                  1.82636   0.42301   0.60321
C                  2.94942   0.41854   1.40791
```

C	4.05457	-0.31841	0.98101
C	3.99916	-1.01957	-0.2252
C	2.86248	-1.0083	-1.03045
H	2.9687	0.97042	2.34256
H	4.95399	-0.34465	1.58569
H	4.86529	-1.5891	-0.54766
H	2.82439	-1.55146	-1.96771
B	-0.32223	0.80407	-0.57675
O	0.59621	-0.16971	-1.25038
C	-1.73408	0.13457	-0.20522
C	-2.83323	0.93536	0.13549
C	-1.90962	-1.25434	-0.16095
C	-4.0553	0.37944	0.50581
H	-2.72775	2.01792	0.10346
C	-3.12715	-1.82233	0.20644
H	-1.07661	-1.89809	-0.43104
C	-4.20404	-1.00495	0.54271
H	-4.89119	1.02338	0.76407
H	-3.23964	-2.90253	0.22872
H	-5.15463	-1.44496	0.82902
O	-0.35536	2.09558	-1.18328
H	-1.04615	2.14126	-1.8463
H	0.66819	2.1145	0.90682
N	0.56397	1.10323	0.8282
H	0.08418	0.76934	1.6621

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	1.80856	0.59486	0.31762
C	1.89077	-0.62377	-0.36689
C	3.06718	-1.03309	-0.96614
C	4.18166	-0.1941	-0.87447
C	4.10114	1.01279	-0.18461
C	2.91311	1.42383	0.42448
H	3.12251	-1.98157	-1.4913
H	5.11538	-0.49002	-1.34035
H	4.97677	1.65071	-0.11888
H	2.83963	2.36537	0.95631
B	-0.27031	-0.28509	0.57065
O	0.57497	0.85227	0.81149
C	-1.76892	-0.00759	0.13263
C	-2.66405	-1.05296	-0.13434
C	-2.23818	1.30259	-0.01314

C	-3.97568	-0.80608	-0.52836
H	-2.33445	-2.08812	-0.04146
C	-3.54909	1.56023	-0.40268
H	-1.55753	2.12542	0.18431
C	-4.42117	0.50616	-0.66118
H	-4.64936	-1.63282	-0.73296
H	-3.89235	2.58514	-0.50723
H	-5.44394	0.70551	-0.96588
O	-0.18398	-1.31717	1.8048
H	-1.04563	-1.65361	2.07272
H	0.33992	-1.85842	0.89997
N	0.62896	-1.28775	-0.28555
H	0.27797	-1.66584	-1.15749

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! R18   R(13,14)        1.4019   1.4027   1.402  -DE/DX =    0.0         !
! R19   R(13,15)        1.3993   1.4019   1.4007 -DE/DX =    0.0         !
! R20   R(14,16)        1.3916   1.3908   1.3927 -DE/DX =    0.0         !
! R21   R(14,17)        1.0903   1.0878   1.0882 -DE/DX =    0.0         !
! R22   R(15,18)        1.3916   1.3901   1.3928 -DE/DX =    0.0         !
! R23   R(15,19)        1.086    1.0858   1.0869 -DE/DX =    0.0         !
! R24   R(16,20)        1.3921   1.3923   1.3928 -DE/DX =    0.0         !
! R25   R(16,21)        1.0859   1.0854   1.0863 -DE/DX =    0.0         !
! R26   R(18,20)        1.3923   1.3928   1.3932 -DE/DX =    0.0         !
! R27   R(18,22)        1.0859   1.0853   1.0863 -DE/DX =    0.0         !
! R28   R(20,23)        1.0857   1.0856   1.0859 -DE/DX =    0.0         !
! R29   R(24,25)        0.963    0.9615   0.9586 -DE/DX =    0.0         !
! R30   R(24,26)        1.1773   0.9615   2.3273 -DE/DX =    0.0         !
! R31   R(26,27)        1.3471   2.4574   1.0197 -DE/DX =    0.0         !
! R32   R(27,28)        1.0131   1.0056   1.0184 -DE/DX =    0.0         !
! A1    A(2,1,6)       120.7826  122.1529  119.0737 -DE/DX =    0.0        !
! A2    A(2,1,12)       113.4177  110.6872  115.1192 -DE/DX =    0.0        !
! A3    A(6,1,12)       125.7904  127.1597  125.804  -DE/DX =    0.0        !
! A4    A(1,2,3)        121.3094  120.769   122.9289 -DE/DX =    0.0        !
! A5    A(1,2,27)       108.9615  106.7018  108.8873 -DE/DX =    0.0        !
! A6    A(3,2,27)       129.7152  132.5286  128.1837 -DE/DX =    0.0        !
! A7    A(2,3,4)        118.1871  117.5028  117.8634 -DE/DX =    0.0        !
! A8    A(2,3,7)        120.7856  121.3958  120.9471 -DE/DX =    0.0        !
! A9    A(4,3,7)        121.0272  121.1013  121.1894 -DE/DX =    0.0        !
! A10   A(3,4,5)        120.4339  121.3259  119.875  -DE/DX =    0.0        !
! A11   A(3,4,8)        119.6288  119.1457  119.952  -DE/DX =    0.0        !
! A12   A(5,4,8)        119.9365  119.528   120.1729 -DE/DX =    0.0        !
! A13   A(4,5,6)        121.3472  121.1351  121.8487 -DE/DX =    0.0        !
! A14   A(4,5,9)        119.5231  119.5164  119.2343 -DE/DX =    0.0        !
! A15   A(6,5,9)        119.1295  119.3485  118.917  -DE/DX =    0.0        !
! A16   A(1,6,5)        117.934   117.1132  118.4102 -DE/DX =    0.0        !
! A17   A(1,6,10)       120.2437  120.7688  119.959  -DE/DX =    0.0        !
! A18   A(5,6,10)       121.8177  122.1179  121.6306 -DE/DX =    0.0        !
! A19   A(12,11,13)     117.6169  122.9461  111.831  -DE/DX =    0.0        !
! A20   A(12,11,24)     110.3052  101.9458  114.2823 -DE/DX =    0.0        !
! A21   A(12,11,26)     118.8983  106.097   114.3172 -DE/DX =    0.0        !
! A22   A(12,11,27)     104.8119  108.1559   99.6464 -DE/DX =    0.0        !
! A23   A(13,11,24)     111.9826   85.0973  117.0716 -DE/DX =    0.0        !
! A24   A(13,11,26)     123.2601   95.9124  119.018  -DE/DX =    0.0        !
! A25   A(13,11,27)     119.6198  128.8967  110.0524 -DE/DX =    0.0        !
! A26   A(1,12,11)      108.9266  107.3216  111.5197 -DE/DX =    0.0        !
! A27   A(11,13,14)     121.7037  121.7416  120.4845 -DE/DX =    0.0        !
! A28   A(11,13,15)     120.6335  120.2103  122.0616 -DE/DX =    0.0        !
! A29   A(14,13,15)     117.6599  118.0437  117.4169 -DE/DX =    0.0        !
! A30   A(13,14,16)     121.5639  121.2036  121.6396 -DE/DX =    0.0        !
! A31   A(13,14,17)     119.9145  119.9291  119.0194 -DE/DX =    0.0        !
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! A32   A(16,14,17)     118.5202  118.8646  119.34   -DE/DX =    0.0         !
! A33   A(13,15,18)     121.2257  121.0384  121.4848 -DE/DX =    0.0         !
! A34   A(13,15,19)     118.7054  119.1416  118.9089 -DE/DX =    0.0         !
! A35   A(18,15,19)     120.0689  119.8199  119.6028 -DE/DX =    0.0         !
! A36   A(14,16,20)     119.7256  119.7706  119.834  -DE/DX =    0.0         !
! A37   A(14,16,21)     120.1996  120.056   120.1192 -DE/DX =    0.0         !
! A38   A(20,16,21)     120.0748  120.1734  120.0468 -DE/DX =    0.0         !
! A39   A(15,18,20)     120.1228  119.9744  120.007  -DE/DX =    0.0         !
! A40   A(15,18,22)     119.9636  120.0024  120.0962 -DE/DX =    0.0         !
! A41   A(20,18,22)     119.9135  120.023   119.8966 -DE/DX =    0.0         !
! A42   A(16,20,18)     119.7013  119.9676  119.6176 -DE/DX =    0.0         !
! A43   A(16,20,23)     120.0879  120.0163  120.2123 -DE/DX =    0.0         !
! A44   A(18,20,23)     120.2108  120.0157  120.1698 -DE/DX =    0.0         !
! A45   A(11,24,25)     112.89     67.187   110.7193 -DE/DX =    0.0         !
! A46   A(25,24,26)     116.8301  103.7035  159.6699 -DE/DX =    0.0         !
! A47   A(11,26,24)      64.4434  113.0162   36.5297 -DE/DX =    0.0         !
! A48   A(24,26,27)     125.2457  145.5843   82.9774 -DE/DX =    0.0         !
! A49   A(2,27,11)      103.6682  107.1254  104.1555 -DE/DX =    0.0         !
! A50   A(2,27,26)      115.8903  103.5897  112.8191 -DE/DX =    0.0         !
! A51   A(2,27,28)      115.504   121.7619  112.5214 -DE/DX =    0.0         !
! A52   A(11,27,28)     120.064   130.5359  112.0949 -DE/DX =    0.0         !
! A53   A(26,27,28)     121.6674   94.8434  108.07   -DE/DX =    0.0         !
! D1    D(6,1,2,3)       -0.5827   -0.3826    0.0527 -DE/DX =    0.0         !
! D2    D(6,1,2,27)     178.1874  179.3584 -179.8601 -DE/DX =    0.0         !
! D3    D(12,1,2,3)     178.37    179.5143  179.4546 -DE/DX =    0.0         !
! D4    D(12,1,2,27)     -2.8599   -0.7446   -0.4582 -DE/DX =    0.0         !
! D5    D(2,1,6,5)        0.767     0.2583   -0.0046 -DE/DX =    0.0         !
! D6    D(2,1,6,10)     179.9942 -179.6091 -179.865  -DE/DX =    0.0         !
! D7    D(12,1,6,5)    -178.0483 -179.6207 -179.3369 -DE/DX =    0.0         !
! D8    D(12,1,6,10)      1.1789    0.5119    0.8027 -DE/DX =    0.0         !
! D9    D(2,1,12,11)      4.7909    0.2604    6.0854 -DE/DX =    0.0         !
! D10   D(6,1,12,11)   -176.3183 -179.8491 -174.5592 -DE/DX =    0.0         !
! D11   D(1,2,3,4)       -0.1223    0.1917   -0.0455 -DE/DX =    0.0         !
! D12   D(1,2,3,7)      179.749  -179.8041 -179.9698 -DE/DX =    0.0         !
! D13   D(27,2,3,4)    -178.6101 -179.4718  179.8496 -DE/DX =    0.0         !
! D14   D(27,2,3,7)       1.2612    0.5324   -0.0747 -DE/DX =    0.0         !
! D15   D(1,2,27,11)     -0.1196    0.9106   -4.5371 -DE/DX =    0.0         !
! D16   D(1,2,27,26)     -75.2918  -82.356  -120.3011 -DE/DX =    0.0         !
! D17   D(1,2,27,28)     133.2929  173.0584  117.0994 -DE/DX =    0.0         !
! D18   D(3,2,27,11)     178.5143 -179.3913  175.556  -DE/DX =    0.0         !
! D19   D(3,2,27,26)     103.3421   97.3421   59.792  -DE/DX =    0.0         !
! D20   D(3,2,27,28)     -48.0732   -7.2435  -62.8075 -DE/DX =    0.0         !
! D21   D(2,3,4,5)        0.6151    0.1001   -0.0089 -DE/DX =    0.0         !
! D22   D(2,3,4,8)     -179.7004  179.8843  179.939  -DE/DX =    0.0         !
! D23   D(7,3,4,5)     -179.2558 -179.9041  179.9152 -DE/DX =    0.0         !
! D24   D(7,3,4,8)        0.4287   -0.1198   -0.1368 -DE/DX =    0.0         !
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! D25   D(3,4,5,6)       -0.4244   -0.2192    0.0565 -DE/DX =    0.0         !
! D26   D(3,4,5,9)       179.7252  179.7635  179.9632 -DE/DX =    0.0         !
! D27   D(8,4,5,6)      -180.1079  179.9974 -179.8914 -DE/DX =    0.0         !
! D28   D(8,4,5,9)        0.0416   -0.02      0.0154 -DE/DX =    0.0         !
! D29   D(4,5,6,1)       -0.2726    0.038    -0.049  -DE/DX =    0.0         !
! D30   D(4,5,6,10)     -179.4869  179.9035  179.809  -DE/DX =    0.0         !
! D31   D(9,5,6,1)       179.5785 -179.9447 -179.9561 -DE/DX =    0.0         !
! D32   D(9,5,6,10)        0.3642   -0.0792   -0.0981 -DE/DX =    0.0         !
! D33   D(13,11,12,1)   -140.1474  179.9274 -124.2276 -DE/DX =    0.0         !
! D34   D(24,11,12,1)     89.7599   88.0354   99.8354 -DE/DX =    0.0         !
! D35   D(26,11,12,1)     45.1197   71.5801   14.7505 -DE/DX =    0.0         !
! D36   D(27,11,12,1)     -4.4791    0.3205   -7.9477 -DE/DX =    0.0         !
! D37   D(12,11,13,14)  -180.5148 -172.1591 -164.886  -DE/DX =    0.0         !
! D38   D(12,11,13,15)     0.1242    7.0631   17.3858 -DE/DX =    0.0         !
! D39   D(24,11,13,14)   -51.2034  -71.0914  -30.2775 -DE/DX =    0.0         !
! D40   D(24,11,13,15)   129.4356  108.1308  151.9943 -DE/DX =    0.0         !
! D41   D(26,11,13,14)    -6.0301  -58.626    58.2693 -DE/DX =    0.0         !
! D42   D(26,11,13,15)   174.6089  120.5962 -119.4589 -DE/DX =    0.0         !
! D43   D(27,11,13,14)    50.485     7.361    85.3357 -DE/DX =    0.0         !
! D44   D(27,11,13,15)  -128.876   -173.4169  -92.3926 -DE/DX =    0.0         !
! D45   D(12,11,24,25)   135.9517  120.6814   91.0906 -DE/DX =    0.0         !
! D46   D(13,11,24,25)     2.921    -1.9874  -42.4399 -DE/DX =    0.0         !
! D47   D(12,11,26,24)    88.3767   77.5317  110.6678 -DE/DX =    0.0         !
! D48   D(13,11,26,24)   -86.0411  -49.2633 -113.4984 -DE/DX =    0.0         !
! D49   D(12,11,27,2)      2.7485   -0.7745    7.2833 -DE/DX =    0.0         !
! D50   D(12,11,27,28)  -128.0024 -171.983  -114.6356 -DE/DX =    0.0         !
! D51   D(13,11,27,2)    137.3287  179.6493  124.9021 -DE/DX =    0.0         !
! D52   D(13,11,27,28)     6.5778    8.4408    2.9832 -DE/DX =    0.0         !
! D53   D(11,13,14,16)  -179.5056  179.3821 -177.7768 -DE/DX =    0.0         !
! D54   D(11,13,14,17)     0.0483   -0.0136    2.5764 -DE/DX =    0.0         !
! D55   D(15,13,14,16)    -0.1264    0.1438    0.0543 -DE/DX =    0.0         !
! D56   D(15,13,14,17)   179.4276 -179.252  -179.5924 -DE/DX =    0.0         !
! D57   D(11,13,15,18)   179.7101 -179.6627  177.8082 -DE/DX =    0.0         !
! D58   D(11,13,15,19)    -0.2989    0.2452   -2.8755 -DE/DX =    0.0         !
! D59   D(14,13,15,18)     0.3239   -0.4122    0.0137 -DE/DX =    0.0         !
! D60   D(14,13,15,19)  -179.6852  179.4957  179.3299 -DE/DX =    0.0         !
! D61   D(13,14,16,20)    -0.1346    0.2122   -0.0201 -DE/DX =    0.0         !
! D62   D(13,14,16,21)   179.7811 -179.7886 -179.9388 -DE/DX =    0.0         !
! D63   D(17,14,16,20)  -179.6945  179.6143  179.6256 -DE/DX =    0.0         !
! D64   D(17,14,16,21)     0.2211   -0.3866   -0.2931 -DE/DX =    0.0         !
! D65   D(13,15,18,20)    -0.2611    0.3239   -0.1157 -DE/DX =    0.0         !
! D66   D(13,15,18,22)   179.8586 -179.8112  179.7183 -DE/DX =    0.0         !
! D67   D(19,15,18,20)   179.7481 -179.5835 -179.4273 -DE/DX =    0.0         !
! D68   D(19,15,18,22)    -0.1322    0.2814    0.4067 -DE/DX =    0.0         !
! D69   D(14,16,20,18)     0.2032   -0.3068   -0.0827 -DE/DX =    0.0         !
! D70   D(14,16,20,23)  -179.8521  179.9137 -179.9009 -DE/DX =    0.0         !
```

```
 ! D71   D(21,16,20,18)  -179.7126  179.6941  179.8361 -DE/DX =    0.0         !
 ! D72   D(21,16,20,23)    0.2321   -0.0855    0.0178 -DE/DX =    0.0         !
 ! D73   D(15,18,20,16)   -0.0091    0.0423    0.1493 -DE/DX =    0.0         !
 ! D74   D(15,18,20,23)   180.0462  179.8219  179.9676 -DE/DX =    0.0         !
 ! D75   D(22,18,20,16)   179.8713 -179.8225 -179.685  -DE/DX =    0.0         !
 ! D76   D(22,18,20,23)   -0.0734   -0.043    0.1333 -DE/DX =    0.0         !
 ! D77   D(25,24,26,11)   108.1019   44.0877   88.7915 -DE/DX =    0.0         !
 ! D78   D(25,24,26,27)   116.4279   43.1789   95.8113 -DE/DX =    0.0         !
 ! D79   D(24,26,27,2)    87.7536  106.868   108.2765 -DE/DX =    0.0         !
 ! D80   D(24,26,27,28)  -122.7357 -128.8007 -126.6666 -DE/DX =    0.0         !
 ---------------------------------------------------------------------------

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradG
radGrad

**********************************************
 %nprocshared=2
 Will use up to    2 processors via shared memory.
 %mem=1GB
 %chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\BOAB
new\FREQ-QS
 T3-TS1-BOAB-N-B-3-29-MIRROR IMAGE-TRIAL 3-CA-WITH INI TSA.chk
 ----------------------
 # freq wb97xd/6-31g(d,p)
 ----------------------
 1/10=4,30=1,38=1/1,3;
 2/12=2,17=6,18=5,40=1/2;
 3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
 4//1;
 5/5=2,38=5,98=1/2;
 8/6=4,10=90,11=11/1;
 11/6=1,8=1,9=11,15=111,16=1/1,2,10;
 10/6=1/2;
 6/7=2,8=2,9=2,10=2,18=1,28=1/1;
 7/8=1,10=1,25=1/1,2,3,16;
 1/10=4,30=1/3;
 99//99;
 ------------------
 Title Card Required
 ------------------
 Symbolic Z-matrix:
 Charge =  0 Multiplicity = 1
 C                  1.80856   0.59486   0.31762
 C                  1.89077  -0.62377  -0.36689
 C                  3.06718  -1.03309  -0.96614
 C                  4.18166  -0.1941   -0.87447
```

C	4.10114	1.01279	-0.18461
C	2.91311	1.42383	0.42448
H	3.12251	-1.98157	-1.4913
H	5.11538	-0.49002	-1.34035
H	4.97677	1.65071	-0.11888
H	2.83963	2.36537	0.95631
B	-0.27031	-0.28509	0.57065
O	0.57497	0.85227	0.81149
C	-1.76892	-0.00759	0.13263
C	-2.66405	-1.05296	-0.13434
C	-2.23818	1.30259	-0.01314
C	-3.97568	-0.80608	-0.52836
H	-2.33445	-2.08812	-0.04146
C	-3.54909	1.56023	-0.40268
H	-1.55753	2.12542	0.18431
C	-4.42117	0.50616	-0.66118
H	-4.64936	-1.63282	-0.73296
H	-3.89235	2.58514	-0.50723
H	-5.44394	0.70551	-0.96588
O	-0.18398	-1.31717	1.8048
H	-1.04563	-1.65361	2.07272
H	0.33992	-1.85842	0.89997
N	0.62896	-1.28775	-0.28555
H	0.27797	-1.66584	-1.15749

GradGradGradG

Sum of electronic and thermal Energies= -694.181426
Sum of electronic and thermal Enthalpies= -694.180482
Sum of electronic and thermal Free Energies= -694.233554

IRC-TS1-A

%nprocshared=2
Will use up to 2 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\BOAB new\IRC of-
OPT-QST3-TS1-BOAB-N-B-3-29-MIRROR IMAGE-TRIAL 3-CA-WITH INI TSA.chk
---
irc=(maxpoints=15,calcfc) wb97xd/6-31g(d,p)

1/10=4,14=-1,18=10,26=3,38=1,42=15,44=3/1,23;
2/12=2,17=6,18=5,29=1,40=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
4//1;
5/5=2,38=5/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1,13=1/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7/10=1,18=20,25=1/1,2,3,16;
1/10=4,14=-1,18=10,26=3,42=15,44=3/23(2);
2/29=1/2;
99/5=20/99;
2/29=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1,13=1/2;
7/10=1,18=20,25=1/1,2,3,16;
1/14=-1,18=10,26=3,42=15,44=3/23(-8);
2/29=1/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/5=20,9=1/99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	1.80856	0.59486	0.31762
C	1.89077	-0.62377	-0.36689
C	3.06718	-1.03309	-0.96614
C	4.18166	-0.1941	-0.87447
C	4.10114	1.01279	-0.18461
C	2.91311	1.42383	0.42448
H	3.12251	-1.98157	-1.4913
H	5.11538	-0.49002	-1.34035
H	4.97677	1.65071	-0.11888
H	2.83963	2.36537	0.95631
B	-0.27031	-0.28509	0.57065
O	0.57497	0.85227	0.81149
C	-1.76892	-0.00759	0.13263
C	-2.66405	-1.05296	-0.13434
C	-2.23818	1.30259	-0.01314
C	-3.97568	-0.80608	-0.52836
H	-2.33445	-2.08812	-0.04146
C	-3.54909	1.56023	-0.40268
H	-1.55753	2.12542	0.18431
C	-4.42117	0.50616	-0.66118
H	-4.64936	-1.63282	-0.73296
H	-3.89235	2.58514	-0.50723
H	-5.44394	0.70551	-0.96588
O	-0.18398	-1.31717	1.8048
H	-1.04563	-1.65361	2.07272
H	0.33992	-1.85842	0.89997
N	0.62896	-1.28775	-0.28555
H	0.27797	-1.66584	-1.15749

IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC

INPUT DATA FOR L123

GENERAL PARAMETERS:
Follow reaction path in both directions.
Maximum points per path = 15
Step size = 0.100 bohr
Integration scheme = HPC
Redo corrector integration= Yes
DWI Weight Power = 2
DWI will use Hessian update vectors when possible.
Max correction cycles = 20
Initial Hessian = CalcFC
Hessian evaluation = All updating
Hessian updating method = Bofill

```
 ---------------------------------------------------------------------
 IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-
IRC-IRC

%nprocshared=5
 Will use up to    5 processors via shared memory.
 %mem=1GB
 %chk=T:\CHM\deg013\Thusini\Reproducing data of li et. al paper\BDAB-
product form
 ation\TPH-01-46--QST3-OPT-BOAB-N-B break-Product formation-1st-GAS
PHASE-8-18.ch
 k
 ---------------------------------------------------------
 # opt=(calcall,qst3) wb97xd/6-31g(d,p) geom=connectivity
 ---------------------------------------------------------
 1/5=1,10=4,14=-1,18=20,26=3,27=203,38=1,57=2/1,3;
 2/9=110,12=2,17=6,18=5,40=1/2;
 3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
 4//1;
 5/5=2,38=5/2;
 8/6=4,10=90,11=11/1;
 11/6=1,8=1,9=11,15=111,16=1/1,2,10;
 10/6=1/2;
 6/7=2,8=2,9=2,10=2,18=1,28=1/1;
 7/10=1,25=1/1,2,3,16;
 1/5=1,10=4,14=-1,18=20,26=3,27=203/3(3);
 2/9=110/2;
 7/8=1,9=1,25=1,44=-1/16;
 99//99;
 2/9=110/2;
 3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
 4/5=5,16=3,69=1/1;
 5/5=2,38=5/2;
 8/6=4,10=90,11=11/1;
 11/6=1,8=1,9=11,15=111,16=1/1,2,10;
 10/6=1/2;
 7/10=1,25=1/1,2,3,16;
 1/5=1,10=4,14=-1,18=20,26=3,27=203/3(-8);
 2/9=110/2;
 6/7=2,8=2,9=2,10=2,18=1,19=2,28=1/1;
 7/8=1,9=1,25=1,44=-1/16;
 99//99;
 ----------------------
 Title Card Required
 ----------------------
 Symbolic Z-matrix:
```

Charge = 0 Multiplicity = 1

C	-0.9875	1.15	0.
C	-1.72563	2.31787	-0.24906
C	-3.10416	2.28927	-0.03349
C	-3.72703	1.13102	0.42141
C	-2.9864	-0.01999	0.66601
C	-1.60993	-0.00722	0.44965
H	-3.68711	3.18722	-0.21775
H	-4.79987	1.13265	0.58296
H	-3.47062	-0.92403	1.01766
H	-1.00482	-0.89316	0.61385
C	2.78946	1.32462	0.44672
C	3.75476	1.46499	1.45161
C	3.22494	1.19489	-0.87794
C	5.1107	1.47864	1.14523
H	3.43428	1.56687	2.48439
C	4.57938	1.20583	-1.19166
H	2.48917	1.08257	-1.66919
C	5.52376	1.34902	-0.17857
H	5.84688	1.59101	1.93511
H	4.90037	1.10311	-2.22375
H	6.58252	1.35975	-0.41976
B	1.27351	1.30924	0.79524
O	0.86191	1.37165	2.09868
H	-0.09363	1.28884	2.19137
O	1.069	4.26069	1.27066
H	0.1932	4.16244	0.86998
H	1.08859	3.60108	1.97025
N	-1.04591	3.4771	-0.63458
H	-0.18046	3.28486	-1.12433
H	-1.61578	4.1494	-1.12802
O	0.3643	1.18415	-0.24492

Add virtual bond connecting atoms N28 and H26 Dist= 3.90D+00.
Add virtual bond connecting atoms H29 and H26 Dist= 4.18D+00.

Title Card Required

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-2.39306	0.08501	-0.17929
C	-1.31121	-0.1953	-1.03337
C	-0.74899	-1.47193	-1.01086
C	-1.27125	-2.45647	-0.17713
C	-2.36036	-2.1831	0.64327
C	-2.91575	-0.90373	0.64257

H	0.11999	-1.68177	-1.62847
H	-0.81604	-3.44152	-0.17038
H	-2.77027	-2.9522	1.2891
H	-3.75669	-0.64884	1.27922
C	1.58002	0.64996	0.43162
C	2.32826	0.53082	-0.74701
C	1.6489	-0.40037	1.35384
C	3.10216	-0.59504	-1.00443
H	2.27544	1.31702	-1.49713
C	2.42687	-1.52844	1.11104
H	1.0876	-0.34219	2.28388
C	3.15123	-1.62952	-0.07235
H	3.66338	-0.67067	-1.93089
H	2.46256	-2.32985	1.84209
H	3.75186	-2.51205	-0.26967
B	0.63737	1.89451	0.66031
O	0.93701	3.14953	0.22267
H	1.80519	3.19323	-0.18113
O	-0.53867	1.78677	1.36564
H	-2.27092	1.9262	0.25944
H	-0.74261	0.86817	1.56804
N	-0.785	0.8501	-1.7924
H	-0.25205	0.55503	-2.59668
H	-1.47682	1.55244	-2.01872
O	-2.92253	1.35525	-0.17966

Add virtual bond connecting atoms H26 and O25 Dist= 3.89D+00.

Title Card Required

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-1.7911	0.12038	-0.17576
C	-2.52923	1.28825	-0.42482
C	-3.90776	1.25964	-0.20925
C	-4.53064	0.10139	0.24565
C	-3.79	-1.04962	0.49025
C	-2.41354	-1.03684	0.27389
H	-4.49072	2.15759	-0.39351
H	-5.60348	0.10303	0.4072
H	-4.27422	-1.95365	0.8419
H	-1.80842	-1.92278	0.43809
C	1.99744	0.17922	0.19167
C	2.96274	0.31959	1.19656
C	2.43292	0.04949	-1.133
C	4.31868	0.33324	0.89017

H	2.64226	0.42146	2.22934
C	3.78736	0.06043	-1.44672
H	1.69715	-0.06283	-1.92424
C	4.73174	0.20362	-0.43362
H	5.05486	0.44561	1.68005
H	4.10835	-0.04229	-2.4788
H	5.7905	0.21435	-0.67482
B	0.48149	0.16384	0.54018
O	0.06989	0.22625	1.84362
H	-0.88565	0.14344	1.93632
O	0.39962	2.14416	0.87443
H	-0.55422	1.65571	0.29731
H	0.41921	1.48455	1.57402
N	-1.84952	2.44747	-0.81034
H	-0.98407	2.25523	-1.30009
H	-2.41938	3.11977	-1.30378
O	-0.4393	0.15453	-0.42068

GradGradGradG

```
! R8    R(4,5)          1.3899    1.3904    1.3907 -DE/DX =    0.0         !
! R9    R(4,8)          1.085     1.0849    1.0852 -DE/DX =    0.0         !
! R10   R(5,6)          1.3927    1.3934    1.3947 -DE/DX =    0.0         !
! R11   R(5,9)          1.0847    1.0842    1.0847 -DE/DX =    0.0         !
! R12   R(6,10)         1.0855    1.0854    1.0851 -DE/DX =    0.0         !
! R13   R(11,12)        1.4016    1.4005    1.4011 -DE/DX =    0.0         !
! R14   R(11,13)        1.3996    1.4004    1.3994 -DE/DX =    0.0         !
! R15   R(11,22)        1.5863    1.5556    1.5779 -DE/DX =    0.0         !
! R16   R(12,14)        1.3915    1.3902    1.3902 -DE/DX =    0.0         !
! R17   R(12,15)        1.088     1.0861    1.0879 -DE/DX =    0.0         !
! R18   R(13,16)        1.392     1.3903    1.3917 -DE/DX =    0.0         !
! R19   R(13,17)        1.0857    1.0863    1.0879 -DE/DX =    0.0         !
! R20   R(14,18)        1.3921    1.3928    1.3933 -DE/DX =    0.0         !
! R21   R(14,19)        1.0859    1.0856    1.0858 -DE/DX =    0.0         !
! R22   R(16,18)        1.392     1.3924    1.3912 -DE/DX =    0.0         !
! R23   R(16,20)        1.086     1.0857    1.0853 -DE/DX =    0.0         !
! R24   R(18,21)        1.0858    1.0859    1.0856 -DE/DX =    0.0         !
! R25   R(22,23)        1.3955    1.3683    1.3625 -DE/DX =    0.0         !
! R26   R(22,25)        1.5449    2.9965    1.3756 -DE/DX =    0.0         !
! R27   R(22,31)        1.6705    1.3872    3.6972 -DE/DX =    0.0         !
! R28   R(23,24)        0.9578    0.9636    0.9585 -DE/DX =    0.0         !
! R29   R(25,26)        1.212     0.9681    2.0601 -DE/DX =    0.0         !
! R30   R(25,27)        0.965     0.9617    0.9625 -DE/DX =    0.0         !
! R31   R(26,28)        2.5281    2.0661    2.7525 -DE/DX =    0.0         !
! R32   R(26,29)        2.3398    2.2107    3.7568 -DE/DX =    0.0         !
! R33   R(26,31)        1.2174    3.1847    0.9713 -DE/DX =    0.0         !
! R34   R(28,29)        1.0131    1.0128    1.0089 -DE/DX =    0.0         !
! R35   R(28,30)        1.011     1.0101    1.0115 -DE/DX =    0.0         !
! A1    A(2,1,6)       121.1491  120.9961  120.4811 -DE/DX =    0.0         !
! A2    A(2,1,31)      118.3974  117.7047  118.6658 -DE/DX =    0.0         !
! A3    A(6,1,31)      120.4475  121.2836  120.8527 -DE/DX =    0.0         !
! A4    A(1,2,3)       118.3085  118.3534  118.85   -DE/DX =    0.0         !
! A5    A(1,2,28)      118.3644  118.8878  118.1116 -DE/DX =    0.0         !
! A6    A(3,2,28)      123.2646  122.674   122.8558 -DE/DX =    0.0         !
! A7    A(2,3,4)       120.7685  120.6438  120.3808 -DE/DX =    0.0         !
! A8    A(2,3,7)       119.1408  119.1392  119.3302 -DE/DX =    0.0         !
! A9    A(4,3,7)       120.0906  120.2152  120.2631 -DE/DX =    0.0         !
! A10   A(3,4,5)       120.203   120.5378  120.5435 -DE/DX =    0.0         !
! A11   A(3,4,8)       119.4894  119.343   119.2383 -DE/DX =    0.0         !
! A12   A(5,4,8)       120.3018  120.1192  120.2178 -DE/DX =    0.0         !
! A13   A(4,5,6)       119.6703  119.4258  119.4647 -DE/DX =    0.0         !
! A14   A(4,5,9)       120.501   120.6262  120.5177 -DE/DX =    0.0         !
! A15   A(6,5,9)       119.8286  119.9474  120.0134 -DE/DX =    0.0         !
! A16   A(1,6,5)       119.873   120.0421  120.2524 -DE/DX =    0.0         !
! A17   A(1,6,10)      118.6959  118.6371  118.1603 -DE/DX =    0.0         !
! A18   A(5,6,10)      121.4311  121.3164  121.5866 -DE/DX =    0.0         !
```

```
! A19   A(12,11,13)     117.6526  118.2727  117.6607 -DE/DX =    0.0         !
! A20   A(12,11,22)     119.2756  120.7932  120.5311 -DE/DX =    0.0         !
! A21   A(13,11,22)     123.0635  120.9339  121.7267 -DE/DX =    0.0         !
! A22   A(11,12,14)     121.5121  121.0064  121.4588 -DE/DX =    0.0         !
! A23   A(11,12,15)     119.325   119.2294  119.5128 -DE/DX =    0.0         !
! A24   A(14,12,15)     119.1627  119.764   118.9862 -DE/DX =    0.0         !
! A25   A(11,13,16)     121.2605  121.04    121.3941 -DE/DX =    0.0         !
! A26   A(11,13,17)     118.9989  119.205   119.8588 -DE/DX =    0.0         !
! A27   A(16,13,17)     119.739   119.7549  118.747  -DE/DX =    0.0         !
! A28   A(12,14,18)     119.8162  119.8561  119.8022 -DE/DX =    0.0         !
! A29   A(12,14,19)     120.0494  120.1389  120.1395 -DE/DX =    0.0         !
! A30   A(18,14,19)     120.1343  120.005   120.0577 -DE/DX =    0.0         !
! A31   A(13,16,18)     120.0907  119.826   119.8931 -DE/DX =    0.0         !
! A32   A(13,16,20)     119.9651  120.1171  119.9603 -DE/DX =    0.0         !
! A33   A(18,16,20)     119.9437  120.0569  120.1456 -DE/DX =    0.0         !
! A34   A(14,18,16)     119.6676  119.9986  119.7866 -DE/DX =    0.0         !
! A35   A(14,18,21)     120.1292  119.9562  120.0968 -DE/DX =    0.0         !
! A36   A(16,18,21)     120.2029  120.0452  120.1166 -DE/DX =    0.0         !
! A37   A(11,22,23)     120.1139  120.4058  123.2701 -DE/DX =    0.0         !
! A38   A(11,22,25)     117.2281   95.2971  121.5536 -DE/DX =    0.0         !
! A39   A(11,22,31)     109.3198  118.1411  115.2935 -DE/DX =    0.0         !
! A40   A(23,22,25)     107.5434   77.4912  115.1418 -DE/DX =    0.0         !
! A41   A(23,22,31)     112.1995  121.4154  105.8504 -DE/DX =    0.0         !
! A42   A(22,23,24)     112.1673  112.7066  112.1174 -DE/DX =    0.0         !
! A43   A(22,25,26)      75.5129   84.0368  115.9932 -DE/DX =    0.0         !
! A44   A(22,25,27)     107.6946   55.8379  111.3292 -DE/DX =    0.0         !
! A45   A(26,25,27)     110.7793  104.4712   89.9621 -DE/DX =    0.0         !
! A46   A(25,26,28)     141.4481  151.3557   85.4047 -DE/DX =    0.0         !
! A47   A(25,26,29)     145.8882  124.5121   86.0811 -DE/DX =    0.0         !
! A48   A(25,26,31)     127.3523  101.0229  140.0937 -DE/DX =    0.0         !
! A49   A(2,28,26)       84.533   111.4589   71.562  -DE/DX =    0.0         !
! A50   A(2,28,29)      112.4975  113.0425  114.4462 -DE/DX =    0.0         !
! A51   A(2,28,30)      112.6293  114.3506  112.5887 -DE/DX =    0.0         !
! A52   A(26,28,30)     161.3919  118.2507   61.7119 -DE/DX =    0.0         !
! A53   A(29,28,30)     109.4899  111.8516  112.7051 -DE/DX =    0.0         !
! A54   A(1,31,22)      120.8     120.8873   76.3563 -DE/DX =    0.0         !
! A55   A(1,31,26)      122.1297   84.7214  106.5203 -DE/DX =    0.0         !
! D1    D(6,1,2,3)        1.5028    0.0087   -1.853  -DE/DX =    0.0         !
! D2    D(6,1,2,28)     178.7222  176.7506 -177.0846 -DE/DX =    0.0         !
! D3    D(31,1,2,3)    -179.3912  178.59    178.3494 -DE/DX =    0.0         !
! D4    D(31,1,2,28)     -2.1718   -4.6681    3.1178 -DE/DX =    0.0         !
! D5    D(2,1,6,5)       -1.6508   -0.277     0.8872 -DE/DX =    0.0         !
! D6    D(2,1,6,10)     178.3971  178.9777 -179.4038 -DE/DX =    0.0         !
! D7    D(31,1,6,5)     179.2614 -178.8072 -179.3197 -DE/DX =    0.0         !
! D8    D(31,1,6,10)     -0.6907    0.4474    0.3893 -DE/DX =    0.0         !
! D9    D(2,1,31,22)     119.9188  102.4631  -57.3188 -DE/DX =    0.0         !
```

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! D10   D(2,1,31,26)     34.6918   37.2934  -71.9428 -DE/DX =    0.0         !
! D11   D(6,1,31,22)    -60.9687  -78.9599  122.8844 -DE/DX =    0.0         !
! D12   D(6,1,31,26)   -146.1956 -144.1296  108.2604 -DE/DX =    0.0         !
! D13   D(1,2,3,4)       -0.0981    0.2116    1.3711 -DE/DX =    0.0         !
! D14   D(1,2,3,7)      179.8127  179.7187 -176.7812 -DE/DX =    0.0         !
! D15   D(28,2,3,4)    -177.1718 -176.3993  176.3637 -DE/DX =    0.0         !
! D16   D(28,2,3,7)       2.739     3.1078   -1.7885 -DE/DX =    0.0         !
! D17   D(1,2,28,26)    -11.5486  -64.9278   17.7864 -DE/DX =    0.0         !
! D18   D(1,2,28,29)     51.5729   28.1383 -159.8065 -DE/DX =    0.0         !
! D19   D(1,2,28,30)    175.8983  157.6678  -29.389  -DE/DX =    0.0         !
! D20   D(3,2,28,26)    165.5235  111.6658 -157.2412 -DE/DX =    0.0         !
! D21   D(3,2,28,29)   -131.3549 -155.2681   25.1659 -DE/DX =    0.0         !
! D22   D(3,2,28,30)     -7.0296  -25.7386  155.5834 -DE/DX =    0.0         !
! D23   D(2,3,4,5)       -1.1522   -0.1653    0.0747 -DE/DX =    0.0         !
! D24   D(2,3,4,8)      179.7175  179.9292 -179.6623 -DE/DX =    0.0         !
! D25   D(7,3,4,5)      178.9379 -179.6671  178.2096 -DE/DX =    0.0         !
! D26   D(7,3,4,8)       -0.1925    0.4274   -1.5273 -DE/DX =    0.0         !
! D27   D(3,4,5,6)        1.0141   -0.1048   -1.0619 -DE/DX =    0.0         !
! D28   D(3,4,5,9)     -179.1041 -179.8196  179.6826 -DE/DX =    0.0         !
! D29   D(8,4,5,6)     -179.8626  179.7999  178.6724 -DE/DX =    0.0         !
! D30   D(8,4,5,9)        0.0191    0.0851   -0.5831 -DE/DX =    0.0         !
! D31   D(4,5,6,1)        0.3718    0.3232    0.5781 -DE/DX =    0.0         !
! D32   D(4,5,6,10)    -179.6775 -178.911  -179.1207 -DE/DX =    0.0         !
! D33   D(9,5,6,1)     -179.5108 -179.96    179.8374 -DE/DX =    0.0         !
! D34   D(9,5,6,10)       0.4399    0.8058    0.1386 -DE/DX =    0.0         !
! D35   D(13,11,12,14)    0.2004    0.1443    0.7063 -DE/DX =    0.0         !
! D36   D(13,11,12,15)  -179.9216  179.9931  178.3197 -DE/DX =    0.0         !
! D37   D(22,11,12,14)   179.1858  179.9679 -176.0668 -DE/DX =    0.0         !
! D38   D(22,11,12,15)    -0.9362   -0.1833    1.5466 -DE/DX =    0.0         !
! D39   D(12,11,13,16)    -0.129    -0.0547   -0.2844 -DE/DX =    0.0         !
! D40   D(12,11,13,17)   179.4017  179.8446  179.5941 -DE/DX =    0.0         !
! D41   D(22,11,13,16)  -179.073  -179.8781  176.4477 -DE/DX =    0.0         !
! D42   D(22,11,13,17)    0.4577    0.0213   -3.6738 -DE/DX =    0.0         !
! D43   D(12,11,22,23)   -39.2808   -2.9965  -35.268  -DE/DX =    0.0         !
! D44   D(12,11,22,25)    94.3751   75.5953  146.9718 -DE/DX =    0.0         !
! D45   D(12,11,22,31)  -171.0544  179.2048   96.9048 -DE/DX =    0.0         !
! D46   D(13,11,22,23)   139.6469  176.8224  148.0924 -DE/DX =    0.0         !
! D47   D(13,11,22,25)   -86.6973 -104.5858  -29.6678 -DE/DX =    0.0         !
! D48   D(13,11,22,31)    7.8732   -0.9763  -79.7349 -DE/DX =    0.0         !
! D49   D(11,12,14,18)    -0.1731   -0.1103   -0.5277 -DE/DX =    0.0         !
! D50   D(11,12,14,19)   179.9929  179.8295  179.1943 -DE/DX =    0.0         !
! D51   D(15,12,14,18)   179.9487 -179.9583 -178.1534 -DE/DX =    0.0         !
! D52   D(15,12,14,19)    0.1148   -0.0185    1.5686 -DE/DX =    0.0         !
! D53   D(11,13,16,18)    0.0314   -0.0684   -0.313  -DE/DX =    0.0         !
! D54   D(11,13,16,20)   179.7698  179.9376 -179.9415 -DE/DX =    0.0         !
! D55   D(17,13,16,18)  -179.4959 -179.9671  179.8071 -DE/DX =    0.0         !
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 ! D56   D(17,13,16,20)    0.2425    0.0388    0.1786 -DE/DX =    0.0         !
 ! D57   D(12,14,18,16)    0.0686   -0.016    -0.0906 -DE/DX =    0.0         !
 ! D58   D(12,14,18,21)  -179.7372  179.9831  179.8341 -DE/DX =    0.0         !
 ! D59   D(19,14,18,16)   179.9024 -179.9559 -179.8129 -DE/DX =    0.0         !
 ! D60   D(19,14,18,21)    0.0966    0.0432    0.1118 -DE/DX =    0.0         !
 ! D61   D(13,16,18,14)    0.0009    0.1043    0.5034 -DE/DX =    0.0         !
 ! D62   D(13,16,18,21)   179.8065 -179.8948 -179.4212 -DE/DX =    0.0         !
 ! D63   D(20,16,18,14)  -179.7376 -179.9017 -179.8688 -DE/DX =    0.0         !
 ! D64   D(20,16,18,21)    0.0681    0.0992    0.2066 -DE/DX =    0.0         !
 ! D65   D(11,22,23,24)   -27.0696 -175.7418   -3.9078 -DE/DX =    0.0         !
 ! D66   D(25,22,23,24)  -164.6378   95.4356  173.9838 -DE/DX =    0.0         !
 ! D67   D(31,22,23,24)   103.4547    1.9837 -139.7564 -DE/DX =    0.0         !
 ! D68   D(11,22,25,26)   116.3118  143.8305 -108.9362 -DE/DX =    0.0         !
 ! D69   D(11,22,25,27)  -136.0994 -104.1742   -8.0068 -DE/DX =    0.0         !
 ! D70   D(23,22,25,26)  -104.7124  -96.1641   73.1324 -DE/DX =    0.0         !
 ! D71   D(23,22,25,27)    2.8764   15.8312  174.0618 -DE/DX =    0.0         !
 ! D72   D(11,22,31,1)   119.1026  179.3073   12.7231 -DE/DX =    0.0         !
 ! D73   D(23,22,31,1)   -16.7287    1.532   152.6219 -DE/DX =    0.0         !
 ! D74   D(22,25,26,31)  -12.1999  -10.3119   95.1336 -DE/DX =    0.0         !
 ! D75   D(27,25,26,28)   27.7854 -101.8261  -84.1242 -DE/DX =    0.0         !
 ! D76   D(27,25,26,29)   67.5273 -107.9454  -85.7085 -DE/DX =    0.0         !
 ! D77   D(27,25,26,31) -115.9521  -62.7189  -18.716  -DE/DX =    0.0         !
 ! D78   D(25,26,28,2)  -126.4564  101.482    86.9054 -DE/DX =    0.0         !
 ! D79   D(25,26,28,30)   31.5253 -122.9441 -143.3598 -DE/DX =    0.0         !
 ! D80   D(25,26,31,1)   126.3808  148.8242  -10.7475 -DE/DX =    0.0         !
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GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradG
radGrad

%nprocshared=2
 Will use up to    2 processors via shared memory.
 %mem=1GB
 %chk=T:\CHM\deg013\Thusini\Reproducing data of li et. al paper\BDAB-
product form
 ation\TPH-01-46--QST3-FREQ-BOAB-N-B                BREAK-PRODUCT
FORMATION-1ST-GAS PHASE-8-18.c
 hk
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 # freq wb97xd/6-31g(d,p) geom=connectivity
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 1/10=4,30=1,38=1,57=2/1,3;
 2/12=2,17=6,18=5,40=1/2;
 3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
 4//1;
 5/5=2,38=5,98=1/2;
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8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1/2;
6/7=2,8=2,9=2,10=2,18=1,28=1/1;
7/8=1,10=1,25=1/1,2,3,16;
1/10=4,30=1/3;
99//99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.63898	-0.16809	-0.28674
C	-2.88879	0.43958	-0.46679
C	-4.0306	-0.28279	-0.12387
C	-3.92998	-1.57626	0.38273
C	-2.68407	-2.17422	0.53086
C	-1.53451	-1.4658	0.19005
H	-5.00686	0.17665	-0.25512
H	-4.8321	-2.11796	0.6472
H	-2.60102	-3.18661	0.91131
H	-0.54754	-1.90673	0.28939
C	2.02408	0.23046	0.10606
C	3.09486	0.22285	1.01038
C	2.22507	-0.36674	-1.14372
C	4.31896	-0.35227	0.68331
H	2.96806	0.67844	1.99022
C	3.44545	-0.94591	-1.47967
H	1.40707	-0.38189	-1.8575
C	4.49582	-0.93991	-0.5662
H	5.13274	-0.34471	1.40232
H	3.57713	-1.40688	-2.45413
H	5.44756	-1.39395	-0.82518
B	0.64561	0.8836	0.5415
O	0.16631	0.70674	1.84011
H	0.48327	-0.10642	2.2347
O	0.41014	2.36086	0.15534
H	-0.44339	1.74946	-0.45009
H	0.03195	2.80785	0.92244
N	-2.92579	1.76939	-0.92842
H	-2.37193	1.90459	-1.76591
H	-3.86779	2.09896	-1.09013
O	-0.51502	0.5449	-0.61127

GradGradGradG

C	3.09486	0.22285	1.01038
C	2.22507	-0.36674	-1.14372
C	4.31896	-0.35227	0.68331
H	2.96806	0.67844	1.99022
C	3.44545	-0.94591	-1.47967
H	1.40707	-0.38189	-1.8575
C	4.49582	-0.93991	-0.5662
H	5.13274	-0.34471	1.40232
H	3.57713	-1.40688	-2.45413
H	5.44756	-1.39395	-0.82518
B	0.64561	0.8836	0.5415
O	0.16631	0.70674	1.84011
H	0.48327	-0.10642	2.2347
O	0.41014	2.36086	0.15534
H	-0.44339	1.74946	-0.45009
H	0.03195	2.80785	0.92244
N	-2.92579	1.76939	-0.92842
H	-2.37193	1.90459	-1.76591
H	-3.86779	2.09896	-1.09013
O	-0.51502	0.5449	-0.61127

GradGradGradG

%chk=T:\CHM\deg013\Thusini\Reproducing data of li et. al paper\BDAB-product form
ation\IRC-TPH-01-46--QST3-OPT-BOAB-N-B BREAK-PRODUCT FORMATION-1ST-GAS PHASE-8-1
8.chk
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irc=calcfc wb97xd/6-31g(d,p) geom=connectivity

1/10=4,14=-1,18=10,26=3,38=1,44=3,57=2/1,23;
2/12=2,17=6,18=5,29=1,40=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
4//1;
5/5=2,38=5/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1,13=1/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7/10=1,18=20,25=1/1,2,3,16;
1/10=4,14=-1,18=10,26=3,44=3/23(2);
2/29=1/2;
99/5=20/99;
2/29=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1,13=1/2;
7/10=1,18=20,25=1/1,2,3,16;
1/14=-1,18=10,26=3,44=3/23(-8);
2/29=1/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/5=20,9=1/99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.63898	-0.16809	-0.28674
C	-2.88879	0.43958	-0.46679
C	-4.0306	-0.28279	-0.12387
C	-3.92998	-1.57626	0.38273
C	-2.68407	-2.17422	0.53086
C	-1.53451	-1.4658	0.19005
H	-5.00686	0.17665	-0.25512
H	-4.8321	-2.11796	0.6472

H	-2.60102	-3.18661	0.91131
H	-0.54754	-1.90673	0.28939
C	2.02408	0.23046	0.10606
C	3.09486	0.22285	1.01038
C	2.22507	-0.36674	-1.14372
C	4.31896	-0.35227	0.68331
H	2.96806	0.67844	1.99022
C	3.44545	-0.94591	-1.47967
H	1.40707	-0.38189	-1.8575
C	4.49582	-0.93991	-0.5662
H	5.13274	-0.34471	1.40232
H	3.57713	-1.40688	-2.45413
H	5.44756	-1.39395	-0.82518
B	0.64561	0.8836	0.5415
O	0.16631	0.70674	1.84011
H	0.48327	-0.10642	2.2347
O	0.41014	2.36086	0.15534
H	-0.44339	1.74946	-0.45009
H	0.03195	2.80785	0.92244
N	-2.92579	1.76939	-0.92842
H	-2.37193	1.90459	-1.76591
H	-3.86779	2.09896	-1.09013
O	-0.51502	0.5449	-0.61127

IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC

Path B - BOAB-H_2O (3.4B)

%mem=1GB
%chk=C:\Users\Dell\Desktop\TPH-01-46-OPT-BOAB-W1-gas phase.chk
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opt wb97xd/6-31g(d,p) geom=connectivity

1/14=-1,18=20,19=15,26=3,38=1,57=2/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4//1;
5/5=2,38=5/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(2);
2/9=110/2;
99//99;
2/9=110/2;

3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	1.98977	0.86535	0.02789
C	1.89204	-0.4786	-0.34981
C	3.00157	-1.27509	-0.54786
C	4.25227	-0.68102	-0.35657
C	4.36202	0.65859	0.01819
C	3.23151	1.45475	0.2171
H	2.89724	-2.31439	-0.8378
H	5.15008	-1.27186	-0.50234
H	5.34537	1.0947	0.15945
H	3.32232	2.49568	0.50856
B	-0.19701	0.28713	-0.17563
C	-1.74865	0.24807	-0.21968
C	-2.40896	-0.89252	-0.70212
C	-2.53085	1.32247	0.22713
C	-3.79823	-0.9584	-0.73691
H	-1.82302	-1.73655	-1.05531
C	-3.91992	1.26364	0.19312
H	-2.05162	2.21729	0.61549
C	-4.5554	0.12172	-0.28975
H	-4.28999	-1.84909	-1.11476
H	-4.50784	2.10522	0.54536
H	-5.6395	0.07292	-0.31619
N	0.68841	1.35349	0.13661
H	0.49828	2.30725	0.39301
O	-0.55298	-1.71968	2.16046
H	-1.44504	-1.51604	1.86367
H	-0.08487	-1.89878	1.33789
O	0.57696	-0.84409	-0.4804

Add virtual bond connecting atoms O28 and H27 Dist= 4.16D+00.

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! R27	R(23,24)	1.0048	-DE/DX = 0.0	!
! R28	R(25,26)	0.9616	-DE/DX = 0.0	!
! R29	R(25,27)	0.9624	-DE/DX = 0.0	!
! R30	R(27,28)	2.267	-DE/DX = 0.0	!
! A1	A(2,1,6)	120.4921	-DE/DX = 0.0	!
! A2	A(2,1,23)	106.9062	-DE/DX = 0.0	!
! A3	A(6,1,23)	132.6014	-DE/DX = 0.0	!
! A4	A(1,2,3)	122.4008	-DE/DX = 0.0	!
! A5	A(1,2,28)	110.4839	-DE/DX = 0.0	!
! A6	A(3,2,28)	127.1152	-DE/DX = 0.0	!
! A7	A(2,3,4)	117.0855	-DE/DX = 0.0	!
! A8	A(2,3,7)	120.8508	-DE/DX = 0.0	!
! A9	A(4,3,7)	122.0637	-DE/DX = 0.0	!
! A10	A(3,4,5)	121.002	-DE/DX = 0.0	!
! A11	A(3,4,8)	119.4062	-DE/DX = 0.0	!
! A12	A(5,4,8)	119.5918	-DE/DX = 0.0	!
! A13	A(4,5,6)	121.4211	-DE/DX = 0.0	!
! A14	A(4,5,9)	119.4969	-DE/DX = 0.0	!
! A15	A(6,5,9)	119.0819	-DE/DX = 0.0	!
! A16	A(1,6,5)	117.5984	-DE/DX = 0.0	!
! A17	A(1,6,10)	121.3376	-DE/DX = 0.0	!
! A18	A(5,6,10)	121.064	-DE/DX = 0.0	!
! A19	A(12,11,23)	130.2886	-DE/DX = 0.0	!
! A20	A(12,11,28)	121.6532	-DE/DX = 0.0	!
! A21	A(23,11,28)	108.0472	-DE/DX = 0.0	!
! A22	A(11,12,13)	119.9547	-DE/DX = 0.0	!
! A23	A(11,12,14)	122.0396	-DE/DX = 0.0	!
! A24	A(13,12,14)	117.9974	-DE/DX = 0.0	!
! A25	A(12,13,15)	121.12	-DE/DX = 0.0	!
! A26	A(12,13,16)	119.1539	-DE/DX = 0.0	!
! A27	A(15,13,16)	119.7259	-DE/DX = 0.0	!
! A28	A(12,14,17)	121.1788	-DE/DX = 0.0	!
! A29	A(12,14,18)	119.8473	-DE/DX = 0.0	!
! A30	A(17,14,18)	118.9699	-DE/DX = 0.0	!
! A31	A(13,15,19)	119.8951	-DE/DX = 0.0	!
! A32	A(13,15,20)	120.0095	-DE/DX = 0.0	!
! A33	A(19,15,20)	120.0952	-DE/DX = 0.0	!
! A34	A(14,17,19)	119.8849	-DE/DX = 0.0	!
! A35	A(14,17,21)	120.049	-DE/DX = 0.0	!
! A36	A(19,17,21)	120.0656	-DE/DX = 0.0	!
! A37	A(15,19,17)	119.9235	-DE/DX = 0.0	!
! A38	A(15,19,22)	120.0242	-DE/DX = 0.0	!
! A39	A(17,19,22)	120.0521	-DE/DX = 0.0	!
! A40	A(1,23,11)	107.5257	-DE/DX = 0.0	!
! A41	A(1,23,24)	121.9793	-DE/DX = 0.0	!
! A42	A(11,23,24)	130.485	-DE/DX = 0.0	!

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! A43   A(26,25,27)         103.2352       -DE/DX =    0.0             !
! A44   A(25,27,28)         135.0285       -DE/DX =    0.0             !
! A45   A(2,28,11)          107.0302       -DE/DX =    0.0             !
! A46   A(2,28,27)          107.3452       -DE/DX =    0.0             !
! A47   A(11,28,27)          89.4172       -DE/DX =    0.0             !
! D1    D(6,1,2,3)            0.0758      -DE/DX =    0.0             !
! D2    D(6,1,2,28)        -179.9854       -DE/DX =    0.0             !
! D3    D(23,1,2,3)         179.8928       -DE/DX =    0.0             !
! D4    D(23,1,2,28)         -0.1684       -DE/DX =    0.0             !
! D5    D(2,1,6,5)           -0.0972       -DE/DX =    0.0             !
! D6    D(2,1,6,10)         179.9592       -DE/DX =    0.0             !
! D7    D(23,1,6,5)        -179.8593       -DE/DX =    0.0             !
! D8    D(23,1,6,10)          0.1971       -DE/DX =    0.0             !
! D9    D(2,1,23,11)          0.6171       -DE/DX =    0.0             !
! D10   D(2,1,23,24)        179.5826       -DE/DX =    0.0             !
! D11   D(6,1,23,11)       -179.5971       -DE/DX =    0.0             !
! D12   D(6,1,23,24)         -0.6317       -DE/DX =    0.0             !
! D13   D(1,2,3,4)           -0.0044       -DE/DX =    0.0             !
! D14   D(1,2,3,7)          179.8986       -DE/DX =    0.0             !
! D15   D(28,2,3,4)        -179.9325       -DE/DX =    0.0             !
! D16   D(28,2,3,7)          -0.0295       -DE/DX =    0.0             !
! D17   D(1,2,28,11)         -0.3554       -DE/DX =    0.0             !
! D18   D(1,2,28,27)        -95.2041       -DE/DX =    0.0             !
! D19   D(3,2,28,11)        179.5798       -DE/DX =    0.0             !
! D20   D(3,2,28,27)         84.7311       -DE/DX =    0.0             !
! D21   D(2,3,4,5)           -0.0415       -DE/DX =    0.0             !
! D22   D(2,3,4,8)          179.9248       -DE/DX =    0.0             !
! D23   D(7,3,4,5)         -179.9432       -DE/DX =    0.0             !
! D24   D(7,3,4,8)            0.0231       -DE/DX =    0.0             !
! D25   D(3,4,5,6)            0.0175       -DE/DX =    0.0             !
! D26   D(3,4,5,9)          179.9358       -DE/DX =    0.0             !
! D27   D(8,4,5,6)         -179.9487       -DE/DX =    0.0             !
! D28   D(8,4,5,9)           -0.0304       -DE/DX =    0.0             !
! D29   D(4,5,6,1)            0.0524       -DE/DX =    0.0             !
! D30   D(4,5,6,10)         179.9962       -DE/DX =    0.0             !
! D31   D(9,5,6,1)         -179.8663       -DE/DX =    0.0             !
! D32   D(9,5,6,10)           0.0775       -DE/DX =    0.0             !
! D33   D(23,11,12,13)      169.6606       -DE/DX =    0.0             !
! D34   D(23,11,12,14)      -11.4109       -DE/DX =    0.0             !
! D35   D(28,11,12,13)       -8.9814       -DE/DX =    0.0             !
! D36   D(28,11,12,14)      169.9471       -DE/DX =    0.0             !
! D37   D(12,11,23,1)      -179.6272       -DE/DX =    0.0             !
! D38   D(12,11,23,24)        1.5266       -DE/DX =    0.0             !
! D39   D(28,11,23,1)        -0.8429       -DE/DX =    0.0             !
! D40   D(28,11,23,24)     -179.6891       -DE/DX =    0.0             !
! D41   D(12,11,28,2)       179.6442       -DE/DX =    0.0             !
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! D42   D(12,11,28,27)       -72.3749       -DE/DX =    0.0              !
! D43   D(23,11,28,2)         0.7336       -DE/DX =    0.0              !
! D44   D(23,11,28,27)       108.7146       -DE/DX =    0.0              !
! D45   D(11,12,13,15)       179.1167       -DE/DX =    0.0              !
! D46   D(11,12,13,16)        -1.0267       -DE/DX =    0.0              !
! D47   D(14,12,13,15)         0.1454       -DE/DX =    0.0              !
! D48   D(14,12,13,16)      -179.998        -DE/DX =    0.0              !
! D49   D(11,12,14,17)      -179.1233       -DE/DX =    0.0              !
! D50   D(11,12,14,18)         0.1374       -DE/DX =    0.0              !
! D51   D(13,12,14,17)        -0.1747       -DE/DX =    0.0              !
! D52   D(13,12,14,18)       179.086        -DE/DX =    0.0              !
! D53   D(12,13,15,19)        -0.004        -DE/DX =    0.0              !
! D54   D(12,13,15,20)       179.8536       -DE/DX =    0.0              !
! D55   D(16,13,15,19)      -179.8598       -DE/DX =    0.0              !
! D56   D(16,13,15,20)        -0.0022       -DE/DX =    0.0              !
! D57   D(12,14,17,19)         0.0625       -DE/DX =    0.0              !
! D58   D(12,14,17,21)       179.8054       -DE/DX =    0.0              !
! D59   D(18,14,17,19)      -179.2046       -DE/DX =    0.0              !
! D60   D(18,14,17,21)         0.5384       -DE/DX =    0.0              !
! D61   D(13,15,19,17)        -0.1127       -DE/DX =    0.0              !
! D62   D(13,15,19,22)      -179.9603       -DE/DX =    0.0              !
! D63   D(20,15,19,17)      -179.9702       -DE/DX =    0.0              !
! D64   D(20,15,19,22)         0.1822       -DE/DX =    0.0              !
! D65   D(14,17,19,15)         0.0839       -DE/DX =    0.0              !
! D66   D(14,17,19,22)       179.9315       -DE/DX =    0.0              !
! D67   D(21,17,19,15)      -179.659        -DE/DX =    0.0              !
! D68   D(21,17,19,22)         0.1886       -DE/DX =    0.0              !
! D69   D(26,25,27,28)        67.05         -DE/DX =    0.0              !
! D70   D(25,27,28,2)         97.9952       -DE/DX =    0.0              !
! D71   D(25,27,28,11)        -9.6828       -DE/DX =    0.0              !
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GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradG
radGrad

**********************************************
 %mem=1GB
 %chk=C:\Users\Dell\Desktop\TPH-01-46-FREQ-BOAB-W1-GAS PHASE.chk
 ----------------------------------------
 # freq wb97xd/6-31g(d,p) geom=connectivity
 ----------------------------------------
 1/10=4,30=1,38=1,57=2/1,3;
 2/12=2,17=6,18=5,40=1/2;
 3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
 4//1;
 5/5=2,38=5,98=1/2;
```

8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1/2;
6/7=2,8=2,9=2,10=2,18=1,28=1/1;
7/8=1,10=1,25=1/1,2,3,16;
1/10=4,30=1/3;
99//99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	1.9862	0.84971	-0.03824
C	1.88942	-0.51613	-0.32592
C	3.0001	-1.32146	-0.47148
C	4.24974	-0.71538	-0.31906
C	4.35807	0.64523	-0.03322
C	3.22674	1.45109	0.11149
H	2.89588	-2.37741	-0.69282
H	5.14821	-1.31372	-0.42444
H	5.34079	1.09045	0.08118
H	3.31776	2.5091	0.33397
B	-0.19925	0.25257	-0.19733
C	-1.75115	0.20964	-0.2425
C	-2.40687	-0.94137	-0.70404
C	-2.53763	1.28704	0.18775
C	-3.7955	-1.01288	-0.73767
H	-1.81552	-1.78774	-1.04203
C	-3.92606	1.22245	0.15623
H	-2.0609	2.18812	0.56522
C	-4.5568	0.07085	-0.3081
H	-4.28417	-1.91157	-1.10053
H	-4.5173	2.06656	0.49685
H	-5.64077	0.01706	-0.33284
N	0.6837	1.34188	0.03532
H	0.49006	2.30657	0.23896
O	-0.52646	-1.34616	2.3504
H	-1.41598	-1.20394	2.01396
H	-0.05768	-1.70362	1.58964
O	0.57552	-0.89241	-0.43029

GradGradGradG

Initialization pass.
Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run= 2 maximum allowed number of steps= 2.

GradGradGradG

7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.64355	-0.39405	-0.33219
C	-2.68138	0.52607	-0.13194
C	-3.94558	0.09583	0.24599
C	-4.18539	-1.26514	0.42696
C	-3.15871	-2.18323	0.24403
C	-1.89083	-1.74553	-0.13354
H	-4.74038	0.82087	0.40536
H	-5.17472	-1.59984	0.71968
H	-3.3406	-3.24205	0.39151
H	-1.07425	-2.44187	-0.2912
C	1.97644	0.07102	0.10106
C	2.86766	0.3246	1.15052
C	2.43205	-0.70196	-0.97364
C	4.16729	-0.17097	1.13017
H	2.5297	0.92266	1.99209
C	3.73122	-1.19872	-1.00451
H	1.75093	-0.92318	-1.79064
C	4.60245	-0.93261	0.0487
H	4.84412	0.03909	1.95289
H	4.0666	-1.79298	-1.84918
H	5.61548	-1.3239	0.02966
B	0.49456	0.61661	0.14804
O	0.04977	1.18766	1.32504
H	-0.85759	1.49695	1.24946
O	0.63591	2.28264	-1.027
H	-0.15234	2.00865	-1.51551
H	0.35	3.03678	-0.49955
N	-0.43526	0.04513	-0.77581
H	-0.05532	-0.85613	-0.56755
O	-2.33528	1.90592	-0.2773
H	-3.1155	2.40769	-0.52444

Add virtual bond connecting atoms O25 and B22 Dist= 3.86D+00.
Add virtual bond connecting atoms H26 and N28 Dist= 4.00D+00.

GradGradGradG

! R27	R(22,28)	1.4358	-DE/DX = 0.0	!
! R28	R(23,24)	0.9633	-DE/DX = 0.0	!
! R29	R(25,26)	0.9635	-DE/DX = 0.0	!
! R30	R(25,27)	0.9618	-DE/DX = 0.0	!
! R31	R(26,28)	2.9571	-DE/DX = 0.0	!
! R32	R(28,29)	1.0101	-DE/DX = 0.0	!
! R33	R(30,31)	0.9616	-DE/DX = 0.0	!
! A1	A(2,1,6)	117.0056	-DE/DX = 0.0	!
! A2	A(2,1,28)	123.4829	-DE/DX = 0.0	!
! A3	A(6,1,28)	119.4731	-DE/DX = 0.0	!
! A4	A(1,2,3)	121.2216	-DE/DX = 0.0	!
! A5	A(1,2,30)	117.7767	-DE/DX = 0.0	!
! A6	A(3,2,30)	121.0015	-DE/DX = 0.0	!
! A7	A(2,3,4)	120.5847	-DE/DX = 0.0	!
! A8	A(2,3,7)	119.1924	-DE/DX = 0.0	!
! A9	A(4,3,7)	120.2172	-DE/DX = 0.0	!
! A10	A(3,4,5)	119.2166	-DE/DX = 0.0	!
! A11	A(3,4,8)	119.9417	-DE/DX = 0.0	!
! A12	A(5,4,8)	120.8416	-DE/DX = 0.0	!
! A13	A(4,5,6)	119.8742	-DE/DX = 0.0	!
! A14	A(4,5,9)	120.429	-DE/DX = 0.0	!
! A15	A(6,5,9)	119.6952	-DE/DX = 0.0	!
! A16	A(1,6,5)	122.084	-DE/DX = 0.0	!
! A17	A(1,6,10)	118.1612	-DE/DX = 0.0	!
! A18	A(5,6,10)	119.7539	-DE/DX = 0.0	!
! A19	A(12,11,13)	117.7674	-DE/DX = 0.0	!
! A20	A(12,11,22)	120.0871	-DE/DX = 0.0	!
! A21	A(13,11,22)	122.1432	-DE/DX = 0.0	!
! A22	A(11,12,14)	121.2411	-DE/DX = 0.0	!
! A23	A(11,12,15)	119.09	-DE/DX = 0.0	!
! A24	A(14,12,15)	119.6688	-DE/DX = 0.0	!
! A25	A(11,13,16)	121.3714	-DE/DX = 0.0	!
! A26	A(11,13,17)	119.6218	-DE/DX = 0.0	!
! A27	A(16,13,17)	118.9711	-DE/DX = 0.0	!
! A28	A(12,14,18)	119.9833	-DE/DX = 0.0	!
! A29	A(12,14,19)	120.036	-DE/DX = 0.0	!
! A30	A(18,14,19)	119.98	-DE/DX = 0.0	!
! A31	A(13,16,18)	119.8666	-DE/DX = 0.0	!
! A32	A(13,16,20)	120.0404	-DE/DX = 0.0	!
! A33	A(18,16,20)	120.0909	-DE/DX = 0.0	!
! A34	A(14,18,16)	119.762	-DE/DX = 0.0	!
! A35	A(14,18,21)	120.1243	-DE/DX = 0.0	!
! A36	A(16,18,21)	120.1105	-DE/DX = 0.0	!
! A37	A(11,22,23)	117.3474	-DE/DX = 0.0	!
! A38	A(11,22,25)	96.6911	-DE/DX = 0.0	!
! A39	A(11,22,28)	117.7144	-DE/DX = 0.0	!

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! A40   A(23,22,25)          79.447         -DE/DX =    0.0             !
! A41   A(23,22,28)          124.8924       -DE/DX =    0.0             !
! A42   A(25,22,28)          96.3391        -DE/DX =    0.0             !
! A43   A(22,23,24)          112.6659       -DE/DX =    0.0             !
! A44   A(22,25,26)          65.7031        -DE/DX =    0.0             !
! A45   A(22,25,27)          59.3437        -DE/DX =    0.0             !
! A46   A(26,25,27)          102.7427       -DE/DX =    0.0             !
! A47   A(25,26,28)          114.908        -DE/DX =    0.0             !
! A48   A(1,28,22)           134.3434       -DE/DX =    0.0             !
! A49   A(1,28,26)           93.5208        -DE/DX =    0.0             !
! A50   A(1,28,29)           111.3319       -DE/DX =    0.0             !
! A51   A(22,28,26)          67.8114        -DE/DX =    0.0             !
! A52   A(22,28,29)          113.0314       -DE/DX =    0.0             !
! A53   A(26,28,29)          127.0921       -DE/DX =    0.0             !
! A54   A(2,30,31)           109.6713       -DE/DX =    0.0             !
! D1    D(6,1,2,3)           1.1984         -DE/DX =    0.0             !
! D2    D(6,1,2,30)          -178.6187      -DE/DX =    0.0             !
! D3    D(28,1,2,3)          178.9273       -DE/DX =    0.0             !
! D4    D(28,1,2,30)         -0.8898        -DE/DX =    0.0             !
! D5    D(2,1,6,5)           -0.3096        -DE/DX =    0.0             !
! D6    D(2,1,6,10)          -179.9601      -DE/DX =    0.0             !
! D7    D(28,1,6,5)          -178.1339      -DE/DX =    0.0             !
! D8    D(28,1,6,10)         2.2156         -DE/DX =    0.0             !
! D9    D(2,1,28,22)         38.8125        -DE/DX =    0.0             !
! D10   D(2,1,28,26)         -23.2223       -DE/DX =    0.0             !
! D11   D(2,1,28,29)         -155.4986      -DE/DX =    0.0             !
! D12   D(6,1,28,22)         -143.5117      -DE/DX =    0.0             !
! D13   D(6,1,28,26)         154.4535       -DE/DX =    0.0             !
! D14   D(6,1,28,29)         22.1771        -DE/DX =    0.0             !
! D15   D(1,2,3,4)           -1.2361        -DE/DX =    0.0             !
! D16   D(1,2,3,7)           179.6348       -DE/DX =    0.0             !
! D17   D(30,2,3,4)          178.5751       -DE/DX =    0.0             !
! D18   D(30,2,3,7)          -0.5539        -DE/DX =    0.0             !
! D19   D(1,2,30,31)         174.1749       -DE/DX =    0.0             !
! D20   D(3,2,30,31)         -5.6427        -DE/DX =    0.0             !
! D21   D(2,3,4,5)           0.3346         -DE/DX =    0.0             !
! D22   D(2,3,4,8)           -179.6244      -DE/DX =    0.0             !
! D23   D(7,3,4,5)           179.4547       -DE/DX =    0.0             !
! D24   D(7,3,4,8)           -0.5043        -DE/DX =    0.0             !
! D25   D(3,4,5,6)           0.5442         -DE/DX =    0.0             !
! D26   D(3,4,5,9)           -179.9179      -DE/DX =    0.0             !
! D27   D(8,4,5,6)           -179.4971      -DE/DX =    0.0             !
! D28   D(8,4,5,9)           0.0408         -DE/DX =    0.0             !
! D29   D(4,5,6,1)           -0.5553        -DE/DX =    0.0             !
! D30   D(4,5,6,10)          179.0898       -DE/DX =    0.0             !
! D31   D(9,5,6,1)           179.9034       -DE/DX =    0.0             !
```

! D32	D(9,5,6,10)	-0.4515	-DE/DX = 0.0	!
! D33	D(13,11,12,14)	-1.0196	-DE/DX = 0.0	!
! D34	D(13,11,12,15)	178.8669	-DE/DX = 0.0	!
! D35	D(22,11,12,14)	179.5128	-DE/DX = 0.0	!
! D36	D(22,11,12,15)	-0.6007	-DE/DX = 0.0	!
! D37	D(12,11,13,16)	0.6026	-DE/DX = 0.0	!
! D38	D(12,11,13,17)	-177.2026	-DE/DX = 0.0	!
! D39	D(22,11,13,16)	-179.9415	-DE/DX = 0.0	!
! D40	D(22,11,13,17)	2.2533	-DE/DX = 0.0	!
! D41	D(12,11,22,23)	29.9409	-DE/DX = 0.0	!
! D42	D(12,11,22,25)	111.4919	-DE/DX = 0.0	!
! D43	D(12,11,22,28)	-147.7184	-DE/DX = 0.0	!
! D44	D(13,11,22,23)	-149.5027	-DE/DX = 0.0	!
! D45	D(13,11,22,25)	-67.9517	-DE/DX = 0.0	!
! D46	D(13,11,22,28)	32.838	-DE/DX = 0.0	!
! D47	D(11,12,14,18)	0.6401	-DE/DX = 0.0	!
! D48	D(11,12,14,19)	-179.6513	-DE/DX = 0.0	!
! D49	D(15,12,14,18)	-179.2458	-DE/DX = 0.0	!
! D50	D(15,12,14,19)	0.4628	-DE/DX = 0.0	!
! D51	D(11,13,16,18)	0.194	-DE/DX = 0.0	!
! D52	D(11,13,16,20)	-179.2858	-DE/DX = 0.0	!
! D53	D(17,13,16,18)	178.0131	-DE/DX = 0.0	!
! D54	D(17,13,16,20)	-1.4667	-DE/DX = 0.0	!
! D55	D(12,14,18,16)	0.1857	-DE/DX = 0.0	!
! D56	D(12,14,18,21)	179.536	-DE/DX = 0.0	!
! D57	D(19,14,18,16)	-179.5231	-DE/DX = 0.0	!
! D58	D(19,14,18,21)	-0.1728	-DE/DX = 0.0	!
! D59	D(13,16,18,14)	-0.5958	-DE/DX = 0.0	!
! D60	D(13,16,18,21)	-179.9463	-DE/DX = 0.0	!
! D61	D(20,16,18,14)	178.8837	-DE/DX = 0.0	!
! D62	D(20,16,18,21)	-0.4668	-DE/DX = 0.0	!
! D63	D(11,22,23,24)	171.748	-DE/DX = 0.0	!
! D64	D(25,22,23,24)	79.6228	-DE/DX = 0.0	!
! D65	D(28,22,23,24)	-10.7784	-DE/DX = 0.0	!
! D66	D(11,22,25,26)	164.8419	-DE/DX = 0.0	!
! D67	D(11,22,25,27)	-71.8655	-DE/DX = 0.0	!
! D68	D(23,22,25,26)	-78.5018	-DE/DX = 0.0	!
! D69	D(23,22,25,27)	44.7908	-DE/DX = 0.0	!
! D70	D(28,22,25,26)	45.8841	-DE/DX = 0.0	!
! D71	D(28,22,25,27)	169.1766	-DE/DX = 0.0	!
! D72	D(11,22,28,1)	173.5008	-DE/DX = 0.0	!
! D73	D(11,22,28,26)	-114.3103	-DE/DX = 0.0	!
! D74	D(11,22,28,29)	7.9899	-DE/DX = 0.0	!
! D75	D(23,22,28,1)	-3.9643	-DE/DX = 0.0	!
! D76	D(23,22,28,26)	68.2245	-DE/DX = 0.0	!
! D77	D(23,22,28,29)	-169.4753	-DE/DX = 0.0	!

```
! D78   D(25,22,28,1)       -85.5006       -DE/DX =    0.0              !
! D79   D(25,22,28,26)      -13.3118       -DE/DX =    0.0              !
! D80   D(25,22,28,29)      108.9884       -DE/DX =    0.0              !
! D81   D(22,25,26,28)      -22.4569       -DE/DX =    0.0              !
! D82   D(27,25,26,28)      -69.9516       -DE/DX =    0.0              !
! D83   D(25,26,28,1)      -171.0057       -DE/DX =    0.0              !
! D84   D(25,26,28,22)       52.008        -DE/DX =    0.0              !
! D85   D(25,26,28,29)      -50.779        -DE/DX =    0.0              !
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GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradG
radGrad

 ******************************************
 %nprocshared=2
 Will use up to    2 processors via shared memory.
 %mem=1GB
 %chk=T:\CHM\deg013\Thusini\Reproducing data of li et. al paper\BDAB-
product form
 ation\TPH-01-46-FREQ-BOAB-INT-1-W1-O-B BREAK 1ST-GAS PHASE-8-
18.chk
 ----------------------------------------
 # freq wb97xd/6-31g(d,p) geom=connectivity
 ----------------------------------------
 1/10=4,30=1,38=1,57=2/1,3;
 2/12=2,17=6,18=5,40=1/2;
 3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
 4//1;
 5/5=2,38=5,98=1/2;
 8/6=4,10=90,11=11/1;
 11/6=1,8=1,9=11,15=111,16=1/1,2,10;
 10/6=1/2;
 6/7=2,8=2,9=2,10=2,18=1,28=1/1;
 7/8=1,10=1,25=1/1,2,3,16;
 1/10=4,30=1/3;
 99//99;
 ------------------
 Title Card Required
 ------------------
 Symbolic Z-matrix:
 Charge =  0 Multiplicity = 1
 C                 -1.81121  -0.59149  -0.015
 C                 -2.61696   0.55657   0.0267
 C                 -4.00194   0.46263   0.08955
 C                 -4.62735  -0.77845   0.08698
 C                 -3.85067  -1.92928   0.02774
```

C	-2.46649	-1.82802	-0.01646
H	-4.59434	1.37403	0.12656
H	-5.70895	-0.83946	0.13021
H	-4.31814	-2.90772	0.0233
H	-1.8606	-2.72942	-0.04777
C	2.10538	-0.12272	0.23213
C	3.07298	0.14516	1.20944
C	2.52742	-0.74187	-0.95189
C	4.40488	-0.21001	1.02247
H	2.77267	0.64137	2.1279
C	3.85869	-1.09274	-1.15086
H	1.81013	-0.92238	-1.74942
C	4.7999	-0.83219	-0.15899
H	5.13755	0.00191	1.79534
H	4.16406	-1.56116	-2.08149
H	5.84026	-1.10361	-0.31048
B	0.60575	0.28024	0.47662
O	0.36933	1.37098	1.26536
H	-0.55759	1.63323	1.26807
O	0.48163	2.44957	-1.60553
H	-0.37898	2.1568	-1.28626
H	0.97711	2.57898	-0.79145
N	-0.41193	-0.55198	-0.10065
H	-0.04467	-1.39999	-0.50849
O	-1.98905	1.78346	-0.00063
H	-2.64682	2.48252	-0.05918

GradGradGradG

Intermediate – B 3.7B

%nprocshared=4
Will use up to 4 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\Intermediates\Us
ing INT C\INT B-correct BY C-CHANGING OH GROUPS.chk
---
opt freq wb97xd/6-31g(d,p)

1/14=-1,18=20,19=15,26=3,38=1/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4//1;
5/5=2,38=5/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(2);
2/9=110/2;
99//99;
2/9=110/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	1.73691	-0.38745	-0.04635
C	2.4778	0.68422	0.47593
C	3.87013	0.60571	0.45329
C	4.51726	-0.50229	-0.07836
C	3.77521	-1.55345	-0.6094
C	2.38745	-1.49111	-0.58694
H	4.42453	1.44162	0.86584
H	5.60167	-0.54044	-0.08301
H	4.26959	-2.42112	-1.0325
H	1.77855	-2.3017	-0.97302

C	-2.07643	0.10224	-0.12077
C	-3.11598	0.91219	-0.59661
C	-2.42238	-1.0839	0.54185
C	-4.4493	0.56153	-0.41645
H	-2.89945	1.83526	-1.13268
C	-3.75257	-1.44092	0.73008
H	-1.63166	-1.72836	0.91298
C	-4.76823	-0.61714	0.25175
H	-5.2373	1.20445	-0.79543
H	-3.99874	-2.36193	1.24899
H	-5.80794	-0.89274	0.39834
B	-0.56769	0.48108	-0.30002
O	-0.14288	1.71101	-0.75704
O	1.90131	1.77432	1.04609
H	-0.85855	2.32626	-0.92858
H	1.14553	2.0371	0.49917
N	0.36321	-0.45303	0.02743
H	0.23947	-1.2868	-0.51063

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.

tem	Value	Threshold	Converged?
Maximum Force	0.000023	0.000450	YES
RMS Force	0.000005	0.000300	YES
Maximum Displacement	0.001542	0.001800	YES
RMS Displacement	0.000418	0.001200	YES

Predicted change in Energy=-1.879753D-08
Optimization completed.
-- Stationary point found.

! Optimized Parameters !
! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.
! R1	R(1,2)	1.4076	-DE/DX = 0.0 !
! R2	R(1,6)	1.3975	-DE/DX = 0.0 !
! R3	R(1,27)	1.4182	-DE/DX = 0.0 !
! R4	R(2,3)	1.396	-DE/DX = 0.0 !
! R5	R(2,24)	1.3552	-DE/DX = 0.0 !
! R6	R(3,4)	1.3875	-DE/DX = 0.0 !
! R7	R(3,7)	1.0846	-DE/DX = 0.0 !

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! R8    R(4,5)              1.3918        -DE/DX =    0.0             !
! R9    R(4,8)              1.0852        -DE/DX =    0.0             !
! R10   R(5,6)               1.3879        -DE/DX =    0.0             !
! R11   R(5,9)               1.0847        -DE/DX =    0.0             !
! R12   R(6,10)              1.0872        -DE/DX =    0.0             !
! R13   R(11,12)             1.4022        -DE/DX =    0.0             !
! R14   R(11,13)             1.4017        -DE/DX =    0.0             !
! R15   R(11,22)             1.572         -DE/DX =    0.0             !
! R16   R(12,14)             1.391         -DE/DX =    0.0             !
! R17   R(12,15)             1.0884        -DE/DX =    0.0             !
! R18   R(13,16)             1.3909        -DE/DX =    0.0             !
! R19   R(13,17)             1.0874        -DE/DX =    0.0             !
! R20   R(14,18)             1.3919        -DE/DX =    0.0             !
! R21   R(14,19)             1.0855        -DE/DX =    0.0             !
! R22   R(16,18)             1.3924        -DE/DX =    0.0             !
! R23   R(16,20)             1.0855        -DE/DX =    0.0             !
! R24   R(18,21)             1.0855        -DE/DX =    0.0             !
! R25   R(22,23)             1.3884        -DE/DX =    0.0             !
! R26   R(22,27)             1.4093        -DE/DX =    0.0             !
! R27   R(23,25)             0.9595        -DE/DX =    0.0             !
! R28   R(24,26)             0.9716        -DE/DX =    0.0             !
! R29   R(27,28)             1.0097        -DE/DX =    0.0             !
! A1    A(2,1,6)            118.7234       -DE/DX =    0.0             !
! A2    A(2,1,27)            122.8526       -DE/DX =    0.0             !
! A3    A(6,1,27)            118.3545       -DE/DX =    0.0             !
! A4    A(1,2,3)            119.1875       -DE/DX =    0.0             !
! A5    A(1,2,24)            123.4027       -DE/DX =    0.0             !
! A6    A(3,2,24)            117.348        -DE/DX =    0.0             !
! A7    A(2,3,4)            121.3255       -DE/DX =    0.0             !
! A8    A(2,3,7)            117.2384       -DE/DX =    0.0             !
! A9    A(4,3,7)            121.4323       -DE/DX =    0.0             !
! A10   A(3,4,5)             119.7255       -DE/DX =    0.0             !
! A11   A(3,4,8)             119.8236       -DE/DX =    0.0             !
! A12   A(5,4,8)             120.45         -DE/DX =    0.0             !
! A13   A(4,5,6)             119.3486       -DE/DX =    0.0             !
! A14   A(4,5,9)             120.7753       -DE/DX =    0.0             !
! A15   A(6,5,9)             119.8757       -DE/DX =    0.0             !
! A16   A(1,6,5)             121.6807       -DE/DX =    0.0             !
! A17   A(1,6,10)             118.4247       -DE/DX =    0.0             !
! A18   A(5,6,10)             119.8939       -DE/DX =    0.0             !
! A19   A(12,11,13)           117.7267       -DE/DX =    0.0             !
! A20   A(12,11,22)           120.6134       -DE/DX =    0.0             !
! A21   A(13,11,22)           121.6597       -DE/DX =    0.0             !
! A22   A(11,12,14)           121.385        -DE/DX =    0.0             !
! A23   A(11,12,15)           119.7353       -DE/DX =    0.0             !
! A24   A(14,12,15)           118.8678       -DE/DX =    0.0             !
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! A25   A(11,13,16)        121.2689       -DE/DX =    0.0            !
! A26   A(11,13,17)        119.4688       -DE/DX =    0.0            !
! A27   A(16,13,17)        119.2489       -DE/DX =    0.0            !
! A28   A(12,14,18)        119.8374       -DE/DX =    0.0            !
! A29   A(12,14,19)        120.0735       -DE/DX =    0.0            !
! A30   A(18,14,19)        120.0886       -DE/DX =    0.0            !
! A31   A(13,16,18)        119.9583       -DE/DX =    0.0            !
! A32   A(13,16,20)        120.0113       -DE/DX =    0.0            !
! A33   A(18,16,20)        120.0302       -DE/DX =    0.0            !
! A34   A(14,18,16)        119.8223       -DE/DX =    0.0            !
! A35   A(14,18,21)        120.0918       -DE/DX =    0.0            !
! A36   A(16,18,21)        120.0855       -DE/DX =    0.0            !
! A37   A(11,22,23)        120.6749       -DE/DX =    0.0            !
! A38   A(11,22,27)        120.4686       -DE/DX =    0.0            !
! A39   A(23,22,27)        118.8533       -DE/DX =    0.0            !
! A40   A(22,23,25)        112.2285       -DE/DX =    0.0            !
! A41   A(2,24,26)          109.245       -DE/DX =    0.0             !
! A42   A(1,27,22)          132.6295      -DE/DX =    0.0             !
! A43   A(1,27,28)          112.0281      -DE/DX =    0.0             !
! A44   A(22,27,28)         114.8874      -DE/DX =    0.0             !
! D1    D(6,1,2,3)          -0.4603      -DE/DX =    0.0            !
! D2    D(6,1,2,24)       -177.5225       -DE/DX =    0.0            !
! D3    D(27,1,2,3)        176.4561       -DE/DX =    0.0            !
! D4    D(27,1,2,24)        -0.6061       -DE/DX =    0.0            !
! D5    D(2,1,6,5)           0.9672      -DE/DX =    0.0            !
! D6    D(2,1,6,10)       -179.3326       -DE/DX =    0.0            !
! D7    D(27,1,6,5)       -176.0893       -DE/DX =    0.0            !
! D8    D(27,1,6,10)         3.6109       -DE/DX =    0.0             !
! D9    D(2,1,27,22)        39.3639       -DE/DX =    0.0             !
! D10   D(2,1,27,28)      -148.9639       -DE/DX =    0.0              !
! D11   D(6,1,27,22)      -143.709        -DE/DX =    0.0             !
! D12   D(6,1,27,28)        27.9632       -DE/DX =    0.0             !
! D13   D(1,2,3,4)          -0.3977      -DE/DX =    0.0            !
! D14   D(1,2,3,7)        -179.6972       -DE/DX =    0.0            !
! D15   D(24,2,3,4)         176.8413       -DE/DX =    0.0            !
! D16   D(24,2,3,7)          -2.4582       -DE/DX =    0.0             !
! D17   D(1,2,24,26)        -37.5373       -DE/DX =    0.0            !
! D18   D(3,2,24,26)        145.3502       -DE/DX =    0.0            !
! D19   D(2,3,4,5)            0.7719      -DE/DX =    0.0            !
! D20   D(2,3,4,8)         -179.5687       -DE/DX =    0.0            !
! D21   D(7,3,4,5)         -179.958        -DE/DX =    0.0             !
! D22   D(7,3,4,8)           -0.2986       -DE/DX =    0.0            !
! D23   D(3,4,5,6)           -0.2714       -DE/DX =    0.0            !
! D24   D(3,4,5,9)          179.5146       -DE/DX =    0.0            !
! D25   D(8,4,5,6)         -179.9287       -DE/DX =    0.0            !
! D26   D(8,4,5,9)           -0.1426       -DE/DX =    0.0            !
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```
 ! D27   D(4,5,6,1)          -0.6033        -DE/DX =    0.0              !
 ! D28   D(4,5,6,10)         179.7009        -DE/DX =    0.0              !
 ! D29   D(9,5,6,1)          179.6088        -DE/DX =    0.0              !
 ! D30   D(9,5,6,10)         -0.0871        -DE/DX =    0.0              !
 ! D31   D(13,11,12,14)       -0.26         -DE/DX =    0.0              !
 ! D32   D(13,11,12,15)     -178.9878        -DE/DX =    0.0              !
 ! D33   D(22,11,12,14)      179.8897        -DE/DX =    0.0              !
 ! D34   D(22,11,12,15)       1.1619         -DE/DX =    0.0              !
 ! D35   D(12,11,13,16)      -0.0951         -DE/DX =    0.0              !
 ! D36   D(12,11,13,17)     -178.7527        -DE/DX =    0.0              !
 ! D37   D(22,11,13,16)      179.7536        -DE/DX =    0.0              !
 ! D38   D(22,11,13,17)       1.0959         -DE/DX =    0.0              !
 ! D39   D(12,11,22,23)       36.1107        -DE/DX =    0.0              !
 ! D40   D(12,11,22,27)     -143.2326        -DE/DX =    0.0              !
 ! D41   D(13,11,22,23)     -143.7337        -DE/DX =    0.0              !
 ! D42   D(13,11,22,27)       36.9231        -DE/DX =    0.0              !
 ! D43   D(11,12,14,18)        0.3791        -DE/DX =    0.0              !
 ! D44   D(11,12,14,19)     -179.3582        -DE/DX =    0.0              !
 ! D45   D(15,12,14,18)      179.1177        -DE/DX =    0.0              !
 ! D46   D(15,12,14,19)       -0.6196        -DE/DX =    0.0              !
 ! D47   D(11,13,16,18)        0.3294        -DE/DX =    0.0              !
 ! D48   D(11,13,16,20)     -179.4845        -DE/DX =    0.0              !
 ! D49   D(17,13,16,18)      178.9899        -DE/DX =    0.0              !
 ! D50   D(17,13,16,20)       -0.824         -DE/DX =    0.0              !
 ! D51   D(12,14,18,16)       -0.1388        -DE/DX =    0.0              !
 ! D52   D(12,14,18,21)      179.6307        -DE/DX =    0.0              !
 ! D53   D(19,14,18,16)      179.5984        -DE/DX =    0.0              !
 ! D54   D(19,14,18,21)       -0.6321        -DE/DX =    0.0              !
 ! D55   D(13,16,18,14)       -0.2097        -DE/DX =    0.0              !
 ! D56   D(13,16,18,21)     -179.9792        -DE/DX =    0.0              !
 ! D57   D(20,16,18,14)      179.6042        -DE/DX =    0.0              !
 ! D58   D(20,16,18,21)       -0.1653        -DE/DX =    0.0              !
 ! D59   D(11,22,23,25)        8.933         -DE/DX =    0.0              !
 ! D60   D(27,22,23,25)     -171.7132        -DE/DX =    0.0              !
 ! D61   D(11,22,27,1)      -179.8603        -DE/DX =    0.0              !
 ! D62   D(11,22,27,28)        8.6512        -DE/DX =    0.0              !
 ! D63   D(23,22,27,1)         0.7846        -DE/DX =    0.0              !
 ! D64   D(23,22,27,28)     -170.7039        -DE/DX =    0.0              !
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radGrad

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 - Thermochemistry -
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Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.226613 (Hartree/Particle)
Thermal correction to Energy= 0.239836
Thermal correction to Enthalpy= 0.240781
Thermal correction to Gibbs Free Energy= 0.185639
Sum of electronic and zero-point Energies= -694.227008
Sum of electronic and thermal Energies= -694.213785
Sum of electronic and thermal Enthalpies= -694.212841
Sum of electronic and thermal Free Energies= -694.267982

BOAB-TS1-B (TS1-B)

%nprocshared=7
Will use up to 7 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\TS1-checking\TS1
-B\OPT-FREQ-QST3-TS1-B-T2-R and P from IRC1-B-guess early output TS1-B.chk
---
opt=(calcall,qst3) freq wb97xd/6-31g(d,p)

1/5=1,10=4,14=-1,18=20,26=3,27=203,38=1/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
4//1;
5/5=2,38=5/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1/2;
6/7=2,8=2,9=2,10=2,18=1,28=1/1;
7/10=1,25=1/1,2,3,16;
1/5=1,10=4,14=-1,18=20,26=3,27=203/3(3);
2/9=110/2;
7/8=1,9=1,25=1,44=-1/16;
99//99;
2/9=110/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1/2;
7/10=1,25=1/1,2,3,16;
1/5=1,10=4,14=-1,18=20,26=3,27=203/3(-8);

2/9=110/2;
6/7=2,8=2,9=2,10=2,18=1,19=2,28=1/1;
7/8=1,9=1,25=1,44=-1/16;
99//99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	1.84019	-0.42281	-0.66045
C	1.85788	0.30579	0.53989
C	2.97521	-0.47921	-1.45016
C	4.12614	0.18675	-1.01276
C	4.14271	0.88317	0.18981
C	2.9925	0.95044	0.98917
H	2.97117	-1.02579	-2.38808
H	5.02114	0.15185	-1.62579
H	5.04829	1.38595	0.5126
H	2.97772	1.50712	1.92002
B	-0.26798	-0.54911	0.27751
C	-1.78903	-0.12007	0.04478
C	-2.85596	-1.00786	-0.16809
C	-2.06849	1.2515	-0.01503
C	-4.14698	-0.54463	-0.42286
H	-2.68088	-2.08277	-0.14421
C	-3.3525	1.7221	-0.2681
H	-1.26	1.9585	0.14918
C	-4.39666	0.82354	-0.47206
H	-4.95516	-1.25203	-0.58361
H	-3.54043	2.79092	-0.3055
H	-5.40018	1.18877	-0.66778
N	0.57408	-0.97158	-0.84024
H	0.25067	-1.19398	-1.76572
O	-0.28424	-1.76067	1.49589
H	-1.15298	-1.79861	1.91661
H	0.28233	-1.21204	2.0687
O	0.6261	0.30027	1.13645

Add virtual bond connecting atoms O25 and B11 Dist= 3.25D+00.
Add virtual bond connecting atoms H27 and O28 Dist= 3.42D+00.

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	1.81988	-0.42361	-0.65091

C	1.89967	0.3072	0.53915
C	2.96739	-0.47405	-1.447
C	4.11829	0.1858	-1.01234
C	4.15958	0.88902	0.18933
C	3.01698	0.95997	0.98784
H	2.96309	-1.02245	-2.38314
H	5.00934	0.14411	-1.6311
H	5.07036	1.38622	0.50218
H	2.99621	1.51535	1.91926
B	-0.36091	-0.75402	0.33249
C	-1.7958	-0.12728	0.03944
C	-2.86622	-1.00685	-0.16937
C	-2.06364	1.24691	-0.02055
C	-4.15272	-0.54272	-0.42622
H	-2.69191	-2.08058	-0.1269
C	-3.34972	1.72079	-0.26806
H	-1.25628	1.95636	0.14104
C	-4.39745	0.82579	-0.4727
H	-4.96297	-1.24817	-0.5852
H	-3.53637	2.79015	-0.3013
H	-5.40013	1.19506	-0.66533
N	0.574	-0.97141	-0.82723
H	0.25537	-1.16806	-1.76065
O	-0.30534	-1.73241	1.39682
H	-1.16046	-1.81711	1.82304
H	0.676	-0.26795	1.95967
O	0.66342	0.34476	1.20242

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	1.83789	-0.43015	-0.64894
C	1.88362	0.29002	0.55191
C	2.97948	-0.48377	-1.44174
C	4.1296	0.17932	-1.00495
C	4.15489	0.87955	0.19699
C	3.00768	0.94502	0.9971
H	2.97505	-1.03073	-2.37898
H	5.02351	0.14205	-1.61963
H	5.06159	1.38119	0.51631
H	2.99176	1.49505	1.93154
B	-0.31691	-0.66231	0.29054
C	-1.7878	-0.12848	0.04243
C	-2.85341	-1.01488	-0.16325

C	-2.0586	1.244	-0.01189
C	-4.14167	-0.55135	-0.41768
H	-2.67555	-2.08831	-0.12875
C	-3.34384	1.71529	-0.26106
H	-1.24988	1.95118	0.15099
C	-4.38849	0.81723	-0.46586
H	-4.95121	-1.25743	-0.57671
H	-3.53231	2.78411	-0.29575
H	-5.39173	1.18394	-0.66021
N	0.58254	-0.98065	-0.83707
H	0.26705	-1.17866	-1.77089
O	-0.25498	-1.71036	1.46247
H	-1.09815	-1.75864	1.92632
H	0.4261	-0.7272	1.80843
O	0.64803	0.27394	1.19573

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! R10   R(5,6)          1.4001   1.4023   1.3958 -DE/DX =    0.0         !
! R11   R(5,9)          1.0843   1.0849   1.0838 -DE/DX =    0.0         !
! R12   R(6,10)         1.0843   1.0847   1.0846 -DE/DX =    0.0         !
! R13   R(11,12)        1.584    1.5974   1.593  -DE/DX =    0.0         !
! R14   R(11,23)        1.477    1.4618   1.5054 -DE/DX =    0.0         !
! R15   R(11,25)        1.5726   1.7183   1.4468 -DE/DX =    0.0         !
! R16   R(11,28)        1.6217   1.5029   1.7359 -DE/DX =    0.0         !
! R17   R(12,13)        1.4017   1.4042   1.4011 -DE/DX =    0.0         !
! R18   R(12,14)        1.3998   1.401    1.4013 -DE/DX =    0.0         !
! R19   R(13,15)        1.3922   1.3951   1.3916 -DE/DX =    0.0         !
! R20   R(13,16)        1.0885   1.0893   1.0886 -DE/DX =    0.0         !
! R21   R(14,17)        1.3919   1.3908   1.3928 -DE/DX =    0.0         !
! R22   R(14,18)        1.0864   1.0865   1.0869 -DE/DX =    0.0         !
! R23   R(15,19)        1.3919   1.3916   1.391  -DE/DX =    0.0         !
! R24   R(15,20)        1.0858   1.086    1.086  -DE/DX =    0.0         !
! R25   R(17,19)        1.3923   1.3926   1.3931 -DE/DX =    0.0         !
! R26   R(17,21)        1.0859   1.0859   1.086  -DE/DX =    0.0         !
! R27   R(19,22)        1.0857   1.0857   1.0857 -DE/DX =    0.0         !
! R28   R(23,24)        1.0054   1.0053   1.0057 -DE/DX =    0.0         !
! R29   R(25,26)        0.9634   0.966    0.9592 -DE/DX =    0.0         !
! R30   R(25,27)        1.2497   0.9747   1.8505 -DE/DX =    0.0         !
! R31   R(27,28)        1.19     1.8095   0.9742 -DE/DX =    0.0         !
! A1    A(2,1,3)       118.8221  119.9074  117.1709 -DE/DX =    0.0         !
! A2    A(2,1,23)      110.6103  109.0562  111.6931 -DE/DX =    0.0         !
! A3    A(3,1,23)      130.567   131.028   131.1344 -DE/DX =    0.0         !
! A4    A(1,2,6)       123.2979  122.0702  125.0472 -DE/DX =    0.0         !
! A5    A(1,2,28)      111.2029  111.0484  111.4572 -DE/DX =    0.0         !
! A6    A(6,2,28)      125.4865  126.8611  123.4375 -DE/DX =    0.0         !
! A7    A(1,3,4)       118.5965  118.467   118.8491 -DE/DX =    0.0         !
! A8    A(1,3,7)       120.5438  120.6974  120.4311 -DE/DX =    0.0         !
! A9    A(4,3,7)       120.8593  120.8354  120.7186 -DE/DX =    0.0         !
! A10   A(3,4,5)       121.5777  121.2378  122.1177 -DE/DX =    0.0         !
! A11   A(3,4,8)       118.9983  119.0919  118.7534 -DE/DX =    0.0         !
! A12   A(5,4,8)       119.4232  119.6697  119.1284 -DE/DX =    0.0         !
! A13   A(4,5,6)       120.1984  120.4975  119.6662 -DE/DX =    0.0         !
! A14   A(4,5,9)       120.0898  119.9755  120.3673 -DE/DX =    0.0         !
! A15   A(6,5,9)       119.7115  119.5255  119.9648 -DE/DX =    0.0         !
! A16   A(2,6,5)       117.504   117.797   117.1403 -DE/DX =    0.0         !
! A17   A(2,6,10)      120.6147  120.5225  120.647  -DE/DX =    0.0         !
! A18   A(5,6,10)      121.8802  121.6657  122.2078 -DE/DX =    0.0         !
! A19   A(12,11,23)    121.2335  120.9781  118.3269 -DE/DX =    0.0         !
! A20   A(12,11,25)    112.0323  106.4787  115.8485 -DE/DX =    0.0         !
! A21   A(12,11,28)    116.7191  119.8638  112.0048 -DE/DX =    0.0         !
! A22   A(23,11,25)    113.4959  110.1113  116.4372 -DE/DX =    0.0         !
! A23   A(23,11,28)    100.9746  104.9312   96.3733 -DE/DX =    0.0         !
! A24   A(25,11,28)     86.8309   89.9355   92.1042 -DE/DX =    0.0         !
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! A25   A(11,12,13)     120.5789  125.152   117.9434 -DE/DX =    0.0         !
! A26   A(11,12,14)     121.5311  117.3275  124.4612 -DE/DX =    0.0         !
! A27   A(13,12,14)     117.8802  117.4462  117.5951 -DE/DX =    0.0         !
! A28   A(12,13,15)     121.333   121.3916  121.6302 -DE/DX =    0.0         !
! A29   A(12,13,16)     119.6615  119.8957  119.4099 -DE/DX =    0.0         !
! A30   A(15,13,16)     119.0052  118.7107  118.9595 -DE/DX =    0.0         !
! A31   A(12,14,17)     121.1197  121.5464  121.1807 -DE/DX =    0.0         !
! A32   A(12,14,18)     119.1965  118.8262  119.457  -DE/DX =    0.0         !
! A33   A(17,14,18)     119.6831  119.6255  119.358  -DE/DX =    0.0         !
! A34   A(13,15,19)     119.8395  119.9296  119.7987 -DE/DX =    0.0         !
! A35   A(13,15,20)     120.0416  119.961   120.0072 -DE/DX =    0.0         !
! A36   A(19,15,20)     120.1187  120.1094  120.1935 -DE/DX =    0.0         !
! A37   A(14,17,19)     120.1041  120.0374  120.1327 -DE/DX =    0.0         !
! A38   A(14,17,21)     119.8872  119.9418  119.9435 -DE/DX =    0.0         !
! A39   A(19,17,21)     120.0087  120.0207  119.9238 -DE/DX =    0.0         !
! A40   A(15,19,17)     119.7229  119.6479  119.6597 -DE/DX =    0.0         !
! A41   A(15,19,22)     120.0861  120.1937  120.2    -DE/DX =    0.0         !
! A42   A(17,19,22)     120.1908  120.1583  120.1401 -DE/DX =    0.0         !
! A43   A(1,23,11)      111.1578  108.14    114.0276 -DE/DX =    0.0         !
! A44   A(1,23,24)      119.2501  119.9266  119.0065 -DE/DX =    0.0         !
! A45   A(11,23,24)     124.0379  125.6309  123.1247 -DE/DX =    0.0         !
! A46   A(11,25,26)     110.9217  110.1828  110.6322 -DE/DX =    0.0         !
! A47   A(11,25,27)      72.673    90.8206   73.0793 -DE/DX =    0.0         !
! A48   A(26,25,27)     113.0578  106.792   114.0473 -DE/DX =    0.0         !
! A49   A(25,27,28)     128.3018  106.1454  104.7418 -DE/DX =    0.0         !
! A50   A(2,28,11)      105.9052  106.7729  105.4269 -DE/DX =    0.0         !
! A51   A(2,28,27)      113.907   113.5101  109.8258 -DE/DX =    0.0         !
! A52   A(11,28,27)      72.1673   73.0872   89.9461 -DE/DX =    0.0         !
! D1    D(3,1,2,6)       -0.3951   -1.7662   -0.827  -DE/DX =    0.0         !
! D2    D(3,1,2,28)     178.3725  176.7012  176.4719 -DE/DX =    0.0         !
! D3    D(23,1,2,6)     179.8804  179.1731  179.579  -DE/DX =    0.0         !
! D4    D(23,1,2,28)     -1.3521   -2.3595   -3.1221 -DE/DX =    0.0         !
! D5    D(2,1,3,4)        0.2867    0.8251    0.6393 -DE/DX =    0.0         !
! D6    D(2,1,3,7)     -179.8991 -179.041  -179.7413 -DE/DX =    0.0         !
! D7    D(23,1,3,4)     179.9473  179.6482 -179.8615 -DE/DX =    0.0         !
! D8    D(23,1,3,7)      -0.2385   -0.218    -0.2422 -DE/DX =    0.0         !
! D9    D(2,1,23,11)     -1.4439    1.4477   -4.6054 -DE/DX =    0.0         !
! D10   D(2,1,23,24)    153.3336  155.077   154.0331 -DE/DX =    0.0         !
! D11   D(3,1,23,11)    178.8737 -177.473   175.8742 -DE/DX =    0.0         !
! D12   D(3,1,23,24)    -26.3487  -23.8437  -25.4873 -DE/DX =    0.0         !
! D13   D(1,2,6,5)       -0.0054    1.3242    0.1667 -DE/DX =    0.0         !
! D14   D(1,2,6,10)     179.626   179.9468  179.3784 -DE/DX =    0.0         !
! D15   D(28,2,6,5)    -178.5942 -176.8881 -176.8206 -DE/DX =    0.0         !
! D16   D(28,2,6,10)      1.0372    1.7345    2.3911 -DE/DX =    0.0         !
! D17   D(1,2,28,11)      3.2519    2.2089    8.1871 -DE/DX =    0.0         !
! D18   D(1,2,28,27)     80.4257   80.6584  103.8371 -DE/DX =    0.0         !
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! D19   D(6,2,28,11)    -178.0132 -179.4143 -174.4628 -DE/DX =    0.0         !
! D20   D(6,2,28,27)    -100.8395 -100.9648  -78.8128 -DE/DX =    0.0         !
! D21   D(1,3,4,5)        0.2075    0.4711    0.1533 -DE/DX =    0.0         !
! D22   D(1,3,4,8)      179.8888 -179.8049  179.8916 -DE/DX =    0.0         !
! D23   D(7,3,4,5)     -179.6061 -179.6629 -179.465  -DE/DX =    0.0         !
! D24   D(7,3,4,8)        0.0752    0.061     0.2734 -DE/DX =    0.0         !
! D25   D(3,4,5,6)       -0.6183   -0.8987   -0.8348 -DE/DX =    0.0         !
! D26   D(3,4,5,9)      179.5652  179.5488  179.6368 -DE/DX =    0.0         !
! D27   D(8,4,5,6)      179.7017  179.3789  179.4278 -DE/DX =    0.0         !
! D28   D(8,4,5,9)       -0.1149   -0.1736   -0.1006 -DE/DX =    0.0         !
! D29   D(4,5,6,2)        0.5056    0.0003    0.6631 -DE/DX =    0.0         !
! D30   D(4,5,6,10)    -179.1209 -178.6056 -178.5354 -DE/DX =    0.0         !
! D31   D(9,5,6,2)     -179.6772  179.5548 -179.8065 -DE/DX =    0.0         !
! D32   D(9,5,6,10)       0.6964    0.9489    0.995  -DE/DX =    0.0         !
! D33   D(23,11,12,13)   78.7695   77.0326   93.4391 -DE/DX =    0.0         !
! D34   D(23,11,12,14)  -100.0693  -99.7428  -86.7487 -DE/DX =    0.0         !
! D35   D(25,11,12,13)   -59.6828  -49.5381  -51.9634 -DE/DX =    0.0         !
! D36   D(25,11,12,14)   121.4784  133.6865  127.8487 -DE/DX =    0.0         !
! D37   D(28,11,12,13)  -157.5534 -149.2384 -155.8374 -DE/DX =    0.0         !
! D38   D(28,11,12,14)    23.6077   33.9862   23.9747 -DE/DX =    0.0         !
! D39   D(12,11,23,1)    133.9221  139.4394  127.6516 -DE/DX =    0.0         !
! D40   D(12,11,23,24)   -19.4194  -12.291   -29.9913 -DE/DX =    0.0         !
! D41   D(25,11,23,1)    -88.1752  -95.6595  -87.146  -DE/DX =    0.0         !
! D42   D(25,11,23,24)   118.4833  112.6101  115.2112 -DE/DX =    0.0         !
! D43   D(28,11,23,1)      3.137    -0.1275    8.4088 -DE/DX =    0.0         !
! D44   D(28,11,23,24)  -150.2045 -151.8578 -149.234  -DE/DX =    0.0         !
! D45   D(12,11,25,26)    -7.9837  -12.0603   -4.0134 -DE/DX =    0.0         !
! D46   D(12,11,25,27)  -116.6446 -120.3062 -113.9255 -DE/DX =    0.0         !
! D47   D(23,11,25,26)  -149.7854 -144.8983 -150.0828 -DE/DX =    0.0         !
! D48   D(23,11,25,27)   101.5537  106.8558  100.0051 -DE/DX =    0.0         !
! D49   D(28,11,25,26)   109.6214  109.2006  111.735  -DE/DX =    0.0         !
! D50   D(28,11,25,27)     0.9605    0.9547    1.8229 -DE/DX =    0.0         !
! D51   D(12,11,28,2)   -137.3385 -141.3741 -133.6907 -DE/DX =    0.0         !
! D52   D(12,11,28,27)   112.114   108.5158  115.7255 -DE/DX =    0.0         !
! D53   D(23,11,28,2)     -3.7921   -1.2551   -9.6276 -DE/DX =    0.0         !
! D54   D(23,11,28,27)  -114.3397 -111.3652 -120.2114 -DE/DX =    0.0         !
! D55   D(25,11,28,2)    109.536   109.5726  107.2697 -DE/DX =    0.0         !
! D56   D(25,11,28,27)    -1.0115   -0.5375   -3.3142 -DE/DX =    0.0         !
! D57   D(11,12,13,15)  -178.6721 -177.0878  179.7548 -DE/DX =    0.0         !
! D58   D(11,12,13,16)    1.1339    2.3877   -0.0234 -DE/DX =    0.0         !
! D59   D(14,12,13,15)    0.2082   -0.3159   -0.0704 -DE/DX =    0.0         !
! D60   D(14,12,13,16)  -179.9858  179.1596 -179.8486 -DE/DX =    0.0         !
! D61   D(11,12,14,17)   178.87    177.3606 -179.3036 -DE/DX =    0.0         !
! D62   D(11,12,14,18)    -1.4395   -3.1469   -0.0692 -DE/DX =    0.0         !
! D63   D(13,12,14,17)     0.001     0.3313    0.5091 -DE/DX =    0.0         !
! D64   D(13,12,14,18)   179.6914  179.8238  179.7435 -DE/DX =    0.0         !
```

```
 ! D65   D(12,13,15,19)    -0.2518    0.1061   -0.3425 -DE/DX =    0.0         !
 ! D66   D(12,13,15,20)   179.8657 -179.9669  179.9359 -DE/DX =    0.0         !
 ! D67   D(16,13,15,19)   179.941  -179.3754  179.4367 -DE/DX =    0.0         !
 ! D68   D(16,13,15,20)     0.0584    0.5515   -0.2849 -DE/DX =    0.0         !
 ! D69   D(12,14,17,19)    -0.1659   -0.1366   -0.5362 -DE/DX =    0.0         !
 ! D70   D(12,14,17,21)   179.7476  179.7986  179.4438 -DE/DX =    0.0         !
 ! D71   D(18,14,17,19)  -179.8548 -179.6251 -179.7713 -DE/DX =    0.0         !
 ! D72   D(18,14,17,21)     0.0586    0.3101    0.2087 -DE/DX =    0.0         !
 ! D73   D(13,15,19,17)     0.0819    0.1       0.3214 -DE/DX =    0.0         !
 ! D74   D(13,15,19,22)  -179.7681 -179.8615 -179.5483 -DE/DX =    0.0         !
 ! D75   D(20,15,19,17)   179.9644 -179.8268 -179.9576 -DE/DX =    0.0         !
 ! D76   D(20,15,19,22)     0.1143    0.2117    0.1728 -DE/DX =    0.0         !
 ! D77   D(14,17,19,15)     0.1237   -0.0855    0.1101 -DE/DX =    0.0         !
 ! D78   D(14,17,19,22)   179.9735  179.876   179.9798 -DE/DX =    0.0         !
 ! D79   D(21,17,19,15)  -179.7897  179.9794 -179.8699 -DE/DX =    0.0         !
 ! D80   D(21,17,19,22)     0.0602   -0.0591   -0.0002 -DE/DX =    0.0         !
 ! D81   D(11,25,27,28)    -1.6657   -0.8255   -3.358  -DE/DX =    0.0         !
 ! D82   D(26,25,27,28)  -107.553  -112.2172 -108.8777 -DE/DX =    0.0         !
 ! D83   D(25,27,28,2)    -98.3014 -100.3549 -103.7283 -DE/DX =    0.0         !
 ! D84   D(25,27,28,11)     1.6197    0.9864    2.6769 -DE/DX =    0.0         !
 ---------------------------------------------------------------------------

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradG
radGrad

 ------------------
 - Thermochemistry -
 ------------------
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
Zero-point correction=                          0.221326 (Hartree/Particle)
 Thermal correction to Energy=                  0.233899
 Thermal correction to Enthalpy=                0.234843
 Thermal correction to Gibbs Free Energy=       0.181472
 Sum of electronic and zero-point Energies=          -694.182332
 Sum of electronic and thermal Energies=             -694.169760
 Sum of electronic and thermal Enthalpies=           -694.168815
 Sum of electronic and thermal Free Energies=        -694.222187
```

IRC1-B for confirming TS1-B

%nprocshared=3
Will use up to 3 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\TS1-checking\TS1
-B\IRC1- of TS1-B using OPT-FREQ-QST3-TS1-B-T2-R AND P FROM IRC1-B-GUESS EARLY O
UTPUT TS1-B.chk
---
irc=(maxpoints=15,calcfc) wb97xd/6-31g(d,p)

1/10=4,14=-1,18=10,26=3,38=1,42=15,44=3/1,23;
2/12=2,17=6,18=5,29=1,40=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
4//1;
5/5=2,38=5/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1,13=1/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7/10=1,18=20,25=1/1,2,3,16;
1/10=4,14=-1,18=10,26=3,42=15,44=3/23(2);
2/29=1/2;
99/5=20/99;
2/29=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1,13=1/2;
7/10=1,18=20,25=1/1,2,3,16;
1/14=-1,18=10,26=3,42=15,44=3/23(-8);
2/29=1/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/5=20,9=1/99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1
C 1.84076 -0.58582 -0.51158
C 1.88896 0.4441 0.43683
C 2.98447 -0.87169 -1.24973
C 4.1394 -0.12248 -1.01063

C	4.16687	0.88928	-0.05598
C	3.01778	1.18932	0.68544
H	2.9779	-1.66241	-1.99272
H	5.03619	-0.34129	-1.58169
H	5.0785	1.45104	0.11473
H	3.00465	1.98119	1.42602
B	-0.31333	-0.53719	0.45225
C	-1.78958	-0.10596	0.07323
C	-2.8141	-1.05966	-0.00139
C	-2.11105	1.22439	-0.22022
C	-4.11108	-0.70234	-0.35962
H	-2.59637	-2.10269	0.22114
C	-3.40637	1.59003	-0.57494
H	-1.33449	1.98201	-0.16411
C	-4.4091	0.62669	-0.64662
H	-4.88823	-1.45877	-0.41295
H	-3.63445	2.62871	-0.79455
H	-5.42008	0.91041	-0.92276
N	0.58222	-1.1599	-0.54365
H	0.26373	-1.59848	-1.39047
O	-0.24215	-1.21458	1.86967
H	-1.08702	-1.14459	2.32721
H	0.43279	-0.1643	1.92479
O	0.65168	0.61823	1.05544

IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC

BOAB-TS2-B (TS2-B)

%nprocshared=2
Will use up to 2 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thusini\Reproducing data of li et. al paper\BDAB-product form
ation\TPH-01-46-QST3-OPT-BOAB-O-B break-Product formation-1st-GAS PHASE-8-21.chk

---

opt=(calcfc,qst3) wb97xd/6-31g(d,p) geom=connectivity

1/5=1,10=4,14=-1,18=20,26=3,27=203,38=1,57=2/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
4//1;
5/5=2,38=5/2;
8/6=4,10=90,11=11/1;

```
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1,13=1/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7/10=1,18=20,25=1/1,2,3,16;
1/5=1,10=4,14=-1,18=20,26=3,27=203/3(2);
2/9=110/2;
99//99;
2/9=110/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/5=1,14=-1,18=20,26=3,27=203/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;
------------------
Title Card Required
------------------
Symbolic Z-matrix:
Charge =  0 Multiplicity = 1
C                 -1.74279  -0.49249  -0.3419
C                 -2.48092   0.67538  -0.59096
C                 -3.85944   0.64677  -0.37539
C                 -4.48232  -0.51148   0.07951
C                 -3.74168  -1.66249   0.32411
C                 -2.36522  -1.64971   0.10775
H                 -4.4424    1.54472  -0.55965
H                 -5.55516  -0.50984   0.24106
H                 -4.22591  -2.56652   0.67576
H                 -1.76011  -2.53565   0.27196
C                  2.03417  -0.31787   0.10482
C                  2.99947  -0.1775    1.10971
C                  2.46965  -0.4476   -1.21984
C                  4.35541  -0.16385   0.80333
H                  2.67899  -0.07563   2.14249
C                  3.8241   -0.43667  -1.53356
H                  1.73388  -0.55992  -2.01109
C                  4.76848  -0.29347  -0.52046
H                  5.0916   -0.05148   1.59321
H                  4.14509  -0.53938  -2.56564
H                  5.82724  -0.28274  -0.76166
B                  0.51823  -0.33325   0.45334
O                  0.10663  -0.27084   1.75678
H                 -0.84891  -0.35365   1.84947
O                  0.31372   2.6182    0.92876
```

H	-0.56208	2.51995	0.52808
H	0.33331	1.95859	1.62835
N	-0.39099	-0.45834	-0.58682
H	-0.4179	-1.2845	-1.14962
O	-1.78564	1.86113	-0.9853
H	-2.40801	2.48692	-1.36299

Add virtual bond connecting atoms O30 and H26 Dist= 3.88D+00.

Title Card Required

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-2.39306	0.08501	-0.17929
C	-1.31121	-0.1953	-1.03337
C	-0.74899	-1.47193	-1.01086
C	-1.27125	-2.45647	-0.17713
C	-2.36036	-2.1831	0.64327
C	-2.91575	-0.90373	0.64257
H	0.11999	-1.68177	-1.62847
H	-0.81604	-3.44152	-0.17038
H	-2.77027	-2.9522	1.2891
H	-3.75669	-0.64884	1.27922
C	1.58002	0.64996	0.43162
C	2.32826	0.53082	-0.74701
C	1.6489	-0.40037	1.35384
C	3.10216	-0.59504	-1.00443
H	2.27544	1.31702	-1.49713
C	2.42687	-1.52844	1.11104
H	1.0876	-0.34219	2.28388
C	3.15123	-1.62952	-0.07235
H	3.66338	-0.67067	-1.93089
H	2.46256	-2.32985	1.84209
H	3.75186	-2.51205	-0.26967
B	0.63737	1.89451	0.66031
O	0.93701	3.14953	0.22267
H	1.80519	3.19323	-0.18113
O	-0.53867	1.78677	1.36564
H	-0.25205	0.55503	-2.59668
H	-0.74261	0.86817	1.56804
N	-0.785	0.8501	-1.7924
H	-1.47682	1.55244	-2.01872
O	-2.92253	1.35525	-0.17966
H	-2.27092	1.9262	0.25944

Add virtual bond connecting atoms H31 and O25 Dist= 3.89D+00.

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.80126	0.36607	-0.13429
C	-2.53939	1.53394	-0.38335
C	-3.91792	1.50534	-0.16778
C	-4.5408	0.34709	0.28712
C	-3.80016	-0.80393	0.53172
C	-2.4237	-0.79115	0.31536
H	-4.50088	2.40329	-0.35204
H	-5.61363	0.34872	0.44867
H	-4.28438	-1.70796	0.88337
H	-1.81858	-1.67709	0.47956
C	1.99561	0.22356	0.19915
C	2.9609	0.36392	1.20404
C	2.43109	0.09383	-1.12551
C	4.31685	0.37758	0.89766
H	2.64042	0.4658	2.23682
C	3.78553	0.10476	-1.43923
H	1.69531	-0.0185	-1.91676
C	4.72991	0.24796	-0.42614
H	5.05303	0.48995	1.68753
H	4.10652	0.00204	-2.47132
H	5.78867	0.25869	-0.66733
B	0.47966	0.20818	0.54767
O	0.06806	0.27058	1.85111
H	-0.88748	0.18777	1.9438
O	0.40145	2.09983	0.86695
H	-0.55422	1.65571	0.29731
H	0.42104	1.44022	1.56654
N	-0.44946	0.40022	-0.37921
H	-0.5009	-0.36029	-1.0265
O	-1.84412	2.71969	-0.77769
H	-2.46965	3.35392	-1.13556

GradGradGradG

RMS Force 0.000003 0.000300 YES
Maximum Displacement 0.000956 0.001800 YES
RMS Displacement 0.000155 0.001200 YES
Predicted change in Energy=-5.914281D-09
Optimization completed.
-- Stationary point found.

Optimized Parameters
(Angstroms and Degrees)

Name	Definition	TS	Reactant	Product	Derivative Info.
R1	R(1,2)	1.4033	1.4039	1.4066	-DE/DX = 0.0
R2	R(1,6)	1.3921	1.3888	1.3879	-DE/DX = 0.0
R3	R(1,28)	1.417	1.3742	2.4028	-DE/DX = 0.0
R4	R(1,30)	2.3636	2.4404	1.3762	-DE/DX = 0.0
R5	R(2,3)	1.3904	1.3956	1.3951	-DE/DX = 0.0
R6	R(2,28)	2.4385	2.3776	1.3949	-DE/DX = 0.0
R7	R(2,30)	1.3646	1.43	2.3936	-DE/DX = 0.0
R8	R(3,4)	1.3924	1.3916	1.3918	-DE/DX = 0.0
R9	R(3,7)	1.0875	1.0863	1.0866	-DE/DX = 0.0
R10	R(4,5)	1.3885	1.3904	1.3907	-DE/DX = 0.0
R11	R(4,8)	1.0848	1.0849	1.0852	-DE/DX = 0.0
R12	R(5,6)	1.3928	1.3934	1.3947	-DE/DX = 0.0
R13	R(5,9)	1.0845	1.0842	1.0847	-DE/DX = 0.0
R14	R(6,10)	1.0867	1.0854	1.0851	-DE/DX = 0.0
R15	R(11,12)	1.3986	1.4005	1.4011	-DE/DX = 0.0
R16	R(11,13)	1.4022	1.4004	1.3994	-DE/DX = 0.0
R17	R(11,22)	1.6014	1.5556	1.5779	-DE/DX = 0.0
R18	R(12,14)	1.3929	1.3902	1.3902	-DE/DX = 0.0
R19	R(12,15)	1.0876	1.0861	1.0879	-DE/DX = 0.0
R20	R(13,16)	1.3909	1.3903	1.3917	-DE/DX = 0.0
R21	R(13,17)	1.089	1.0863	1.0879	-DE/DX = 0.0
R22	R(14,18)	1.3909	1.3928	1.3933	-DE/DX = 0.0
R23	R(14,19)	1.0862	1.0856	1.0858	-DE/DX = 0.0
R24	R(16,18)	1.3929	1.3924	1.3912	-DE/DX = 0.0
R25	R(16,20)	1.0861	1.0857	1.0853	-DE/DX = 0.0
R26	R(18,21)	1.0858	1.0859	1.0856	-DE/DX = 0.0
R27	R(22,23)	1.4118	1.3683	1.3625	-DE/DX = 0.0
R28	R(22,25)	1.5805	2.9965	1.3756	-DE/DX = 0.0
R29	R(22,28)	1.6429	1.3872	3.0215	-DE/DX = 0.0
R30	R(23,24)	0.9579	0.9636	0.9585	-DE/DX = 0.0
R31	R(25,26)	1.1762	0.9681	4.1592	-DE/DX = 0.0
R32	R(25,27)	0.9662	0.9617	0.9625	-DE/DX = 0.0
R33	R(25,31)	3.6835	3.5605	2.0601	-DE/DX = 0.0
R34	R(26,28)	1.3489	3.1847	1.0089	-DE/DX = 0.0

```
! R35   R(26,30)         2.4083    2.0546    3.6897 -DE/DX =    0.0         !
! R36   R(28,29)         1.0142    1.0       1.0115 -DE/DX =    0.0         !
! R37   R(30,31)         0.9607    0.96      0.9713 -DE/DX =    0.0         !
! A1    A(2,1,6)        118.4816  120.9961  120.4811 -DE/DX =    0.0         !
! A2    A(2,1,28)       119.6796  117.7047   30.8017 -DE/DX =    0.0         !
! A3    A(2,1,30)        30.8736   30.8682  118.6658 -DE/DX =    0.0         !
! A4    A(6,1,28)       121.8344  121.2836  151.2148 -DE/DX =    0.0         !
! A5    A(6,1,30)       149.3285  151.7785  120.8527 -DE/DX =    0.0         !
! A6    A(1,2,3)        120.3087  118.3534  118.85   -DE/DX =    0.0         !
! A7    A(1,2,28)        30.3214   30.7785  118.1116 -DE/DX =    0.0         !
! A8    A(1,2,30)       117.2762  118.8878   30.2959 -DE/DX =    0.0         !
! A9    A(3,2,28)       150.6148  149.1166  122.8558 -DE/DX =    0.0         !
! A10   A(3,2,30)       122.4036  122.674   149.1254 -DE/DX =    0.0         !
! A11   A(2,3,4)        120.4002  120.6438  120.3808 -DE/DX =    0.0         !
! A12   A(2,3,7)        119.4406  119.1392  119.3302 -DE/DX =    0.0         !
! A13   A(4,3,7)        120.1573  120.2152  120.2631 -DE/DX =    0.0         !
! A14   A(3,4,5)        119.8378  120.5378  120.5435 -DE/DX =    0.0         !
! A15   A(3,4,8)        119.6433  119.343   119.2383 -DE/DX =    0.0         !
! A16   A(5,4,8)        120.5186  120.1192  120.2178 -DE/DX =    0.0         !
! A17   A(4,5,6)        119.5867  119.4258  119.4647 -DE/DX =    0.0         !
! A18   A(4,5,9)        120.5297  120.6262  120.5177 -DE/DX =    0.0         !
! A19   A(6,5,9)        119.8817  119.9474  120.0134 -DE/DX =    0.0         !
! A20   A(1,6,5)        121.3787  120.0421  120.2524 -DE/DX =    0.0         !
! A21   A(1,6,10)       118.559   118.6371  118.1603 -DE/DX =    0.0         !
! A22   A(5,6,10)       120.0616  121.3164  121.5866 -DE/DX =    0.0         !
! A23   A(12,11,13)     117.1255  118.2727  117.6607 -DE/DX =    0.0         !
! A24   A(12,11,22)     120.8825  120.7932  120.5311 -DE/DX =    0.0         !
! A25   A(13,11,22)     121.9892  120.9339  121.7267 -DE/DX =    0.0         !
! A26   A(11,12,14)     121.7335  121.0064  121.4588 -DE/DX =    0.0         !
! A27   A(11,12,15)     119.2395  119.2294  119.5128 -DE/DX =    0.0         !
! A28   A(14,12,15)     119.0205  119.764   118.9862 -DE/DX =    0.0         !
! A29   A(11,13,16)     121.7588  121.04    121.3941 -DE/DX =    0.0         !
! A30   A(11,13,17)     119.6497  119.205   119.8588 -DE/DX =    0.0         !
! A31   A(16,13,17)     118.5814  119.7549  118.747  -DE/DX =    0.0         !
! A32   A(12,14,18)     119.9683  119.8561  119.8022 -DE/DX =    0.0         !
! A33   A(12,14,19)     119.9818  120.1389  120.1395 -DE/DX =    0.0         !
! A34   A(18,14,19)     120.0495  120.005   120.0577 -DE/DX =    0.0         !
! A35   A(13,16,18)     119.9     119.826   119.8931 -DE/DX =    0.0         !
! A36   A(13,16,20)     120.096   120.1171  119.9603 -DE/DX =    0.0         !
! A37   A(18,16,20)     120.0037  120.0569  120.1456 -DE/DX =    0.0         !
! A38   A(14,18,16)     119.5054  119.9986  119.7866 -DE/DX =    0.0         !
! A39   A(14,18,21)     120.2953  119.9562  120.0968 -DE/DX =    0.0         !
! A40   A(16,18,21)     120.1985  120.0452  120.1166 -DE/DX =    0.0         !
! A41   A(11,22,23)     119.8057  120.4058  123.2701 -DE/DX =    0.0         !
! A42   A(11,22,25)     111.9943   95.2971  121.5536 -DE/DX =    0.0         !
! A43   A(11,22,28)     110.8402  118.1411   83.7395 -DE/DX =    0.0         !
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! A44   A(23,22,25)     107.1802   77.4912  115.1418 -DE/DX =    0.0         !
! A45   A(23,22,28)     113.5032  121.4154   99.2754 -DE/DX =    0.0         !
! A46   A(22,23,24)     111.8373  112.7066  112.1174 -DE/DX =    0.0         !
! A47   A(22,25,27)     106.4761   55.8379  111.3292 -DE/DX =    0.0         !
! A48   A(22,25,31)      92.7329   85.051   115.9932 -DE/DX =    0.0         !
! A49   A(26,25,27)     106.1752  104.4712   86.1171 -DE/DX =    0.0         !
! A50   A(27,25,31)      43.1548  117.2906   89.9621 -DE/DX =    0.0         !
! A51   A(25,26,30)     102.6214  151.18     42.4249 -DE/DX =    0.0         !
! A52   A(1,28,22)      119.2485  120.8873   83.1163 -DE/DX =    0.0         !
! A53   A(1,28,29)      111.0553   93.0549   85.0421 -DE/DX =    0.0         !
! A54   A(2,28,26)       91.5679   60.4928  114.4462 -DE/DX =    0.0         !
! A55   A(2,28,29)      137.3156  111.6719  112.5887 -DE/DX =    0.0         !
! A56   A(22,28,29)     112.6346  120.9412  105.2832 -DE/DX =    0.0         !
! A57   A(26,28,29)     117.9971  165.5071  112.7051 -DE/DX =    0.0         !
! A58   A(1,30,31)      140.9173  138.0567  106.5203 -DE/DX =    0.0         !
! A59   A(2,30,26)       92.4748  110.6287   30.5309 -DE/DX =    0.0         !
! A60   A(2,30,31)      109.0748  109.5      95.1876 -DE/DX =    0.0         !
! A61   A(26,30,31)     158.4194  117.8293   86.4502 -DE/DX =    0.0         !
! A62   A(25,31,30)      30.9479   43.5502  140.0937 -DE/DX =    0.0         !
! D1    D(6,1,2,3)        0.6554    0.0087   -1.853  -DE/DX =    0.0         !
! D2    D(6,1,2,28)     179.2503 -178.5813 -177.0846 -DE/DX =    0.0         !
! D3    D(6,1,2,30)    -178.1409  176.7506  179.7976 -DE/DX =    0.0         !
! D4    D(28,1,2,3)    -178.5949  178.59    175.2316 -DE/DX =    0.0         !
! D5    D(28,1,2,30)      2.6088   -4.6681   -3.1178 -DE/DX =    0.0         !
! D6    D(30,1,2,3)     178.7963 -176.7419  178.3494 -DE/DX =    0.0         !
! D7    D(30,1,2,28)     -2.6088    4.6681    3.1178 -DE/DX =    0.0         !
! D8    D(2,1,6,5)       -0.0273   -0.277     0.8872 -DE/DX =    0.0         !
! D9    D(2,1,6,10)    -179.7286  178.9777 -179.4038 -DE/DX =    0.0         !
! D10   D(28,1,6,5)     179.206  -178.8072   -2.2133 -DE/DX =    0.0         !
! D11   D(28,1,6,10)     -0.4952    0.4474  177.4957 -DE/DX =    0.0         !
! D12   D(30,1,6,5)      -1.8975    3.2489 -179.3197 -DE/DX =    0.0         !
! D13   D(30,1,6,10)    178.4012 -177.4965    0.3893 -DE/DX =    0.0         !
! D14   D(2,1,28,22)     71.1963  102.4631 -100.9719 -DE/DX =    0.0         !
! D15   D(2,1,28,29)   -155.3139 -128.3462  152.9484 -DE/DX =    0.0         !
! D16   D(6,1,28,22)   -108.0281  -78.9599  -95.7492 -DE/DX =    0.0         !
! D17   D(6,1,28,29)     25.4617   50.2308  158.1711 -DE/DX =    0.0         !
! D18   D(2,1,30,31)      1.5769  -23.4903  -71.9428 -DE/DX =    0.0         !
! D19   D(6,1,30,31)      4.7814  -29.3879  108.2604 -DE/DX =    0.0         !
! D20   D(1,2,3,4)       -0.6259    0.2116    1.3711 -DE/DX =    0.0         !
! D21   D(1,2,3,7)      179.8722  179.7187 -176.7812 -DE/DX =    0.0         !
! D22   D(28,2,3,4)      -2.0716    1.6173  176.3637 -DE/DX =    0.0         !
! D23   D(28,2,3,7)     178.4264 -178.8756   -1.7885 -DE/DX =    0.0         !
! D24   D(30,2,3,4)     178.107  -176.3993    2.9937 -DE/DX =    0.0         !
! D25   D(30,2,3,7)      -1.395     3.1078 -175.1585 -DE/DX =    0.0         !
! D26   D(1,2,28,26)    171.3417 -136.1124 -159.8065 -DE/DX =    0.0         !
! D27   D(1,2,28,29)     35.0929   57.4296  -29.389  -DE/DX =    0.0         !
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! D28   D(3,2,28,26)     173.8145 -138.5303   25.1659 -DE/DX =    0.0         !
! D29   D(3,2,28,29)      37.5657   55.0117  155.5834 -DE/DX =    0.0         !
! D30   D(1,2,30,26)       2.2275  -64.9278 -172.2819 -DE/DX =    0.0         !
! D31   D(1,2,30,31)    -178.9482  163.5828  113.7589 -DE/DX =    0.0         !
! D32   D(3,2,30,26)    -176.5417  111.6658 -175.0999 -DE/DX =    0.0         !
! D33   D(3,2,30,31)       2.2826  -19.8236  110.9408 -DE/DX =    0.0         !
! D34   D(2,3,4,5)        -0.0439   -0.1653    0.0747 -DE/DX =    0.0         !
! D35   D(2,3,4,8)      -179.8521  179.9292 -179.6623 -DE/DX =    0.0         !
! D36   D(7,3,4,5)       179.4545 -179.6671  178.2096 -DE/DX =    0.0         !
! D37   D(7,3,4,8)        -0.3538    0.4274   -1.5273 -DE/DX =    0.0         !
! D38   D(3,4,5,6)         0.6663   -0.1048   -1.0619 -DE/DX =    0.0         !
! D39   D(3,4,5,9)      -179.8315 -179.8196  179.6826 -DE/DX =    0.0         !
! D40   D(8,4,5,6)      -179.5272  179.7999  178.6724 -DE/DX =    0.0         !
! D41   D(8,4,5,9)        -0.025     0.0851   -0.5831 -DE/DX =    0.0         !
! D42   D(4,5,6,1)        -0.6339    0.3232    0.5781 -DE/DX =    0.0         !
! D43   D(4,5,6,10)      179.0629 -178.911  -179.1207 -DE/DX =    0.0         !
! D44   D(9,5,6,1)       179.8607 -179.96    179.8374 -DE/DX =    0.0         !
! D45   D(9,5,6,10)       -0.4425    0.8058    0.1386 -DE/DX =    0.0         !
! D46   D(13,11,12,14)    -0.9829    0.1443    0.7063 -DE/DX =    0.0         !
! D47   D(13,11,12,15)   178.0832  179.9931  178.3197 -DE/DX =    0.0         !
! D48   D(22,11,12,14)   178.416   179.9679 -176.0668 -DE/DX =    0.0         !
! D49   D(22,11,12,15)    -2.5179   -0.1833    1.5466 -DE/DX =    0.0         !
! D50   D(12,11,13,16)     0.8361   -0.0547   -0.2844 -DE/DX =    0.0         !
! D51   D(12,11,13,17)  -177.9905  179.8446  179.5941 -DE/DX =    0.0         !
! D52   D(22,11,13,16)  -178.5556 -179.8781  176.4477 -DE/DX =    0.0         !
! D53   D(22,11,13,17)     2.6178    0.0213   -3.6738 -DE/DX =    0.0         !
! D54   D(12,11,22,23)     1.0706   -2.9965  -35.268  -DE/DX =    0.0         !
! D55   D(12,11,22,25)   127.8334   75.5953  146.9718 -DE/DX =    0.0         !
! D56   D(12,11,22,28)  -134.1506  179.2048   61.7369 -DE/DX =    0.0         !
! D57   D(13,11,22,23)  -179.5602  176.8224  148.0924 -DE/DX =    0.0         !
! D58   D(13,11,22,25)   -52.7974 -104.5858  -29.6678 -DE/DX =    0.0         !
! D59   D(13,11,22,28)    45.2186   -0.9763 -114.9027 -DE/DX =    0.0         !
! D60   D(11,12,14,18)     0.3706   -0.1103   -0.5277 -DE/DX =    0.0         !
! D61   D(11,12,14,19)  -179.8409  179.8295  179.1943 -DE/DX =    0.0         !
! D62   D(15,12,14,18)  -178.6975 -179.9583 -178.1534 -DE/DX =    0.0         !
! D63   D(15,12,14,19)     1.091    -0.0185    1.5686 -DE/DX =    0.0         !
! D64   D(11,13,16,18)    -0.0763   -0.0684   -0.313  -DE/DX =    0.0         !
! D65   D(11,13,16,20)  -179.8645  179.9376 -179.9415 -DE/DX =    0.0         !
! D66   D(17,13,16,18)   178.7624 -179.9671  179.8071 -DE/DX =    0.0         !
! D67   D(17,13,16,20)    -1.0258    0.0388    0.1786 -DE/DX =    0.0         !
! D68   D(12,14,18,16)     0.4266   -0.016    -0.0906 -DE/DX =    0.0         !
! D69   D(12,14,18,21)  -179.8998  179.9831  179.8341 -DE/DX =    0.0         !
! D70   D(19,14,18,16)  -179.3618 -179.9559 -179.8129 -DE/DX =    0.0         !
! D71   D(19,14,18,21)     0.3118    0.0432    0.1118 -DE/DX =    0.0         !
! D72   D(13,16,18,14)    -0.5696    0.1043    0.5034 -DE/DX =    0.0         !
! D73   D(13,16,18,21)   179.7564 -179.8948 -179.4212 -DE/DX =    0.0         !
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 ! D74   D(20,16,18,14)   179.2187 -179.9017 -179.8688 -DE/DX =    0.0         !
 ! D75   D(20,16,18,21)    -0.4552    0.0992    0.2066 -DE/DX =    0.0         !
 ! D76   D(11,22,23,24)   -50.6913 -175.7418   -3.9078 -DE/DX =    0.0         !
 ! D77   D(25,22,23,24)  -179.6584   95.4356  173.9838 -DE/DX =    0.0         !
 ! D78   D(28,22,23,24)    83.432     1.9837  -92.4754 -DE/DX =    0.0         !
 ! D79   D(11,22,25,27)  -144.111  -104.1742   -8.0068 -DE/DX =    0.0         !
 ! D80   D(11,22,25,31)   174.2628  127.8774 -108.9362 -DE/DX =    0.0         !
 ! D81   D(23,22,25,27)   -10.7975   15.8312  174.0618 -DE/DX =    0.0         !
 ! D82   D(23,22,25,31)   -52.4237 -112.1172   73.1324 -DE/DX =    0.0         !
 ! D83   D(11,22,28,1)    131.1525  179.3073  103.6505 -DE/DX =    0.0         !
 ! D84   D(11,22,28,29)    -1.6619   63.7767 -173.4281 -DE/DX =    0.0         !
 ! D85   D(23,22,28,1)     -7.0509    1.532  -133.5792 -DE/DX =    0.0         !
 ! D86   D(23,22,28,29)  -139.8653 -113.9987  -50.6578 -DE/DX =    0.0         !
 ! D87   D(27,25,26,30)    -6.4873 -103.5141   78.5076 -DE/DX =    0.0         !
 ! D88   D(22,25,31,30)   -48.7436   -0.1927   95.1336 -DE/DX =    0.0         !
 ! D89   D(27,25,31,30)  -160.1032  -47.4344  -18.716  -DE/DX =    0.0         !
 ! D90   D(25,26,30,2)   -134.5794  102.9622  -80.2873 -DE/DX =    0.0         !
 ! D91   D(25,26,30,31)    48.4427 -130.0211   26.1826 -DE/DX =    0.0         !
 ! D92   D(1,30,31,25)    155.3515  148.2322  -10.7475 -DE/DX =    0.0         !
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GradGradGradG

6/7=2,8=2,9=2,10=2,18=1,28=1/1;
7/8=1,10=1,25=1/1,2,3,16;
1/10=4,30=1/3;
99//99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.68336	-0.33827	-0.49868
C	-2.69757	0.55139	-0.11239
C	-3.93501	0.06894	0.29883
C	-4.18589	-1.30056	0.31956
C	-3.19517	-2.19041	-0.0735
C	-1.95262	-1.70382	-0.47234
H	-4.71016	0.77095	0.59715
H	-5.15659	-1.66341	0.64033
H	-3.37934	-3.25915	-0.06433
H	-1.16669	-2.39409	-0.76695
C	2.05214	0.20304	0.13048
C	2.74687	-0.23178	1.26376
C	2.7001	0.07184	-1.10606
C	4.01921	-0.79127	1.17322
H	2.28942	-0.11719	2.24376
C	3.97158	-0.48219	-1.21117
H	2.21028	0.42747	-2.01136
C	4.63397	-0.92214	-0.06758
H	4.53197	-1.12187	2.07184
H	4.44929	-0.56881	-2.18269
H	5.62501	-1.359	-0.14448
B	0.57487	0.80879	0.2541
O	-0.03046	0.92857	1.52388
H	0.01269	0.10907	2.0179
O	0.45021	2.2148	-0.45703
H	-0.22376	1.4862	-1.08821
H	-0.15435	2.74177	0.0818
N	-0.41756	0.16659	-0.88691
H	0.06183	-0.48395	-1.49975
O	-2.42008	1.88555	-0.18461
H	-3.1839	2.38205	0.12036

GradGradGradG

Initialization pass.
Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run= 2 maximum allowed number of steps= 2.

GradGradGradG

2/29=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1,13=1/2;
7/10=1,25=1/1,2,3,16;
1/10=4,14=-1,18=10,26=3,42=15,44=3,71=1/23(-8);
2/29=1/2;
6/7=2,8=2,9=2,10=2,18=1,19=2,28=1/1;
99/5=20/99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.68336	-0.33827	-0.49868
C	-2.69757	0.55139	-0.11239
C	-3.93501	0.06894	0.29883
C	-4.18589	-1.30056	0.31956
C	-3.19517	-2.19041	-0.0735
C	-1.95262	-1.70382	-0.47234
H	-4.71016	0.77095	0.59715
H	-5.15659	-1.66341	0.64033
H	-3.37934	-3.25915	-0.06433
H	-1.16669	-2.39409	-0.76695
C	2.05214	0.20304	0.13048
C	2.74687	-0.23178	1.26376
C	2.7001	0.07184	-1.10606
C	4.01921	-0.79127	1.17322
H	2.28942	-0.11719	2.24376
C	3.97158	-0.48219	-1.21117
H	2.21028	0.42747	-2.01136
C	4.63397	-0.92214	-0.06758
H	4.53197	-1.12187	2.07184
H	4.44929	-0.56881	-2.18269
H	5.62501	-1.359	-0.14448
B	0.57487	0.80879	0.2541
O	-0.03046	0.92857	1.52388
H	0.01269	0.10907	2.0179
O	0.45021	2.2148	-0.45703
H	-0.22376	1.4862	-1.08821
H	-0.15435	2.74177	0.0818
N	-0.41756	0.16659	-0.88691
H	0.06183	-0.48395	-1.49975

O -2.42008 1.88555 -0.18461
H -3.1839 2.38205 0.12036

IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC

Benzodioxaborole 3.1C

%nprocshared=1
Will use up to 1 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thusini\Reproducing data of li et. al paper\BDOB-Gas phase-7-
16\BDOB-1st reaction-7-20\BDOB-1st reaction-gas phase-7-20\TPH-01-46-OPT-BDOB-Ga
s phase.chk
---
opt wb97xd/6-31g(d,p) geom=connectivity

1/14=-1,18=20,19=15,26=3,38=1,57=2/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4//1;
5/5=2,38=5/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(2);
2/9=110/2;
99//99;
2/9=110/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1
C 0. 0.69589 -1.85036

C	0.	-0.69589	-1.85036
C	0.	-1.42871	-3.01976
C	0.	-0.69768	-4.21277
C	0.	0.69768	-4.21277
C	0.	1.42871	-3.01976
H	0.	-2.51225	-3.00845
H	0.	-1.23025	-5.15777
H	0.	1.23025	-5.15777
H	0.	2.51225	-3.00845
B	0.	0.	0.231
O	0.	1.14558	-0.55442
O	0.	-1.14558	-0.55442
C	0.	0.	1.77559
C	0.	-1.20521	2.4923
C	0.	1.20521	2.4923
C	0.	-1.20744	3.88275
H	0.	-2.14832	1.95336
C	0.	1.20744	3.88275
H	0.	2.14832	1.95336
C	0.	0.	4.57804
H	0.	-2.14769	4.42492
H	0.	2.14769	4.42492
H	0.	0.	5.66385

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```
! R2    R(1,6)            1.3797       -DE/DX =    0.0001          !
! R3    R(1,12)           1.371        -DE/DX =   -0.0001          !
! R4    R(2,3)            1.3797       -DE/DX =    0.0001          !
! R5    R(2,13)           1.371        -DE/DX =   -0.0001          !
! R6    R(3,4)            1.3986       -DE/DX =    0.0            !
! R7    R(3,7)            1.0835       -DE/DX =    0.0            !
! R8    R(4,5)            1.3949       -DE/DX =    0.0001          !
! R9    R(4,8)            1.0847       -DE/DX =    0.0            !
! R10   R(5,6)            1.3986       -DE/DX =    0.0             !
! R11   R(5,9)            1.0847       -DE/DX =    0.0             !
! R12   R(6,10)           1.0835       -DE/DX =    0.0             !
! R13   R(11,12)          1.3891       -DE/DX =    0.0001          !
! R14   R(11,13)          1.3891       -DE/DX =    0.0001          !
! R15   R(11,14)          1.5443       -DE/DX =    0.0             !
! R16   R(14,15)          1.4015       -DE/DX =    0.0001          !
! R17   R(14,16)          1.4015       -DE/DX =    0.0001          !
! R18   R(15,17)          1.3901       -DE/DX =    0.0             !
! R19   R(15,18)          1.0862       -DE/DX =    0.0             !
! R20   R(16,19)          1.3901       -DE/DX =    0.0             !
! R21   R(16,20)          1.0862       -DE/DX =    0.0             !
! R22   R(17,21)          1.3927       -DE/DX =    0.0001          !
! R23   R(17,22)          1.0854       -DE/DX =    0.0             !
! R24   R(19,21)          1.3927       -DE/DX =    0.0001          !
! R25   R(19,23)          1.0854       -DE/DX =    0.0             !
! R26   R(21,24)          1.0859       -DE/DX =    0.0             !
! A1    A(2,1,6)          122.035      -DE/DX =    0.0             !
! A2    A(2,1,12)         109.158      -DE/DX =    0.0             !
! A3    A(6,1,12)         128.807      -DE/DX =    0.0             !
! A4    A(1,2,3)          122.035      -DE/DX =    0.0             !
! A5    A(1,2,13)         109.158      -DE/DX =    0.0             !
! A6    A(3,2,13)         128.807      -DE/DX =    0.0             !
! A7    A(2,3,4)          116.4908     -DE/DX =    0.0             !
! A8    A(2,3,7)          121.3684     -DE/DX =   -0.0001          !
! A9    A(4,3,7)          122.1408     -DE/DX =    0.0001          !
! A10   A(3,4,5)          121.4742     -DE/DX =    0.0             !
! A11   A(3,4,8)          119.1508     -DE/DX =    0.0             !
! A12   A(5,4,8)          119.375      -DE/DX =    0.0             !
! A13   A(4,5,6)          121.4742     -DE/DX =    0.0             !
! A14   A(4,5,9)          119.375      -DE/DX =    0.0             !
! A15   A(6,5,9)          119.1508     -DE/DX =    0.0             !
! A16   A(1,6,5)          116.4908     -DE/DX =    0.0             !
! A17   A(1,6,10)         121.3684     -DE/DX =   -0.0001          !
! A18   A(5,6,10)         122.1408     -DE/DX =    0.0001          !
! A19   A(12,11,13)       111.1434     -DE/DX =   -0.0001          !
! A20   A(12,11,14)       124.4283     -DE/DX =    0.0             !
! A21   A(13,11,14)       124.4283     -DE/DX =    0.0             !
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! A22   A(1,12,11)        105.2703       -DE/DX =    0.0001          !
! A23   A(2,13,11)        105.2703       -DE/DX =    0.0001          !
! A24   A(11,14,15)       120.7284       -DE/DX =    0.0             !
! A25   A(11,14,16)       120.7284       -DE/DX =    0.0             !
! A26   A(15,14,16)       118.5432       -DE/DX =    0.0             !
! A27   A(14,15,17)       120.8154       -DE/DX =    0.0             !
! A28   A(14,15,18)       119.4317       -DE/DX =    0.0             !
! A29   A(17,15,18)       119.7528       -DE/DX =    0.0             !
! A30   A(14,16,19)       120.8154       -DE/DX =    0.0             !
! A31   A(14,16,20)       119.4317       -DE/DX =    0.0             !
! A32   A(19,16,20)       119.7528       -DE/DX =    0.0             !
! A33   A(15,17,21)       119.8555       -DE/DX =    0.0             !
! A34   A(15,17,22)       120.0553       -DE/DX =    0.0             !
! A35   A(21,17,22)       120.0892       -DE/DX =    0.0             !
! A36   A(16,19,21)       119.8555       -DE/DX =    0.0             !
! A37   A(16,19,23)       120.0553       -DE/DX =    0.0             !
! A38   A(21,19,23)       120.0892       -DE/DX =    0.0             !
! A39   A(17,21,19)       120.115        -DE/DX =    0.0             !
! A40   A(17,21,24)       119.9425       -DE/DX =    0.0             !
! A41   A(19,21,24)       119.9425       -DE/DX =    0.0             !
! D1    D(6,1,2,3)         0.0          -DE/DX =    0.0             !
! D2    D(6,1,2,13)      180.0           -DE/DX =    0.0             !
! D3    D(12,1,2,3)      180.0           -DE/DX =    0.0             !
! D4    D(12,1,2,13)       0.0           -DE/DX =    0.0             !
! D5    D(2,1,6,5)         0.0          -DE/DX =    0.0             !
! D6    D(2,1,6,10)      180.0           -DE/DX =    0.0             !
! D7    D(12,1,6,5)      180.0           -DE/DX =    0.0             !
! D8    D(12,1,6,10)       0.0           -DE/DX =    0.0             !
! D9    D(2,1,12,11)       0.0           -DE/DX =    0.0             !
! D10   D(6,1,12,11)     180.0            -DE/DX =    0.0             !
! D11   D(1,2,3,4)         0.0          -DE/DX =    0.0             !
! D12   D(1,2,3,7)       180.0           -DE/DX =    0.0             !
! D13   D(13,2,3,4)      180.0            -DE/DX =    0.0             !
! D14   D(13,2,3,7)        0.0           -DE/DX =    0.0             !
! D15   D(1,2,13,11)       0.0           -DE/DX =    0.0             !
! D16   D(3,2,13,11)     180.0            -DE/DX =    0.0             !
! D17   D(2,3,4,5)         0.0          -DE/DX =    0.0             !
! D18   D(2,3,4,8)       180.0           -DE/DX =    0.0             !
! D19   D(7,3,4,5)       180.0           -DE/DX =    0.0             !
! D20   D(7,3,4,8)         0.0          -DE/DX =    0.0             !
! D21   D(3,4,5,6)         0.0          -DE/DX =    0.0             !
! D22   D(3,4,5,9)       180.0           -DE/DX =    0.0             !
! D23   D(8,4,5,6)       180.0           -DE/DX =    0.0             !
! D24   D(8,4,5,9)         0.0          -DE/DX =    0.0             !
! D25   D(4,5,6,1)         0.0          -DE/DX =    0.0             !
! D26   D(4,5,6,10)      180.0            -DE/DX =    0.0             !
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! D27   D(9,5,6,1)          180.0          -DE/DX =    0.0             !
! D28   D(9,5,6,10)          0.0          -DE/DX =    0.0             !
! D29   D(13,11,12,1)        0.0           -DE/DX =    0.0             !
! D30   D(14,11,12,1)       180.0           -DE/DX =    0.0             !
! D31   D(12,11,13,2)        0.0          -DE/DX =    0.0             !
! D32   D(14,11,13,2)       180.0           -DE/DX =    0.0             !
! D33   D(12,11,14,15)      180.0           -DE/DX =    0.0             !
! D34   D(12,11,14,16)       0.0           -DE/DX =    0.0             !
! D35   D(13,11,14,15)       0.0           -DE/DX =    0.0             !
! D36   D(13,11,14,16)      180.0           -DE/DX =    0.0             !
! D37   D(11,14,15,17)      180.0           -DE/DX =    0.0             !
! D38   D(11,14,15,18)       0.0           -DE/DX =    0.0             !
! D39   D(16,14,15,17)       0.0           -DE/DX =    0.0             !
! D40   D(16,14,15,18)      180.0           -DE/DX =    0.0             !
! D41   D(11,14,16,19)      180.0           -DE/DX =    0.0             !
! D42   D(11,14,16,20)       0.0           -DE/DX =    0.0             !
! D43   D(15,14,16,19)       0.0           -DE/DX =    0.0             !
! D44   D(15,14,16,20)      180.0           -DE/DX =    0.0             !
! D45   D(14,15,17,21)       0.0           -DE/DX =    0.0             !
! D46   D(14,15,17,22)      180.0           -DE/DX =    0.0             !
! D47   D(18,15,17,21)      180.0           -DE/DX =    0.0             !
! D48   D(18,15,17,22)       0.0           -DE/DX =    0.0             !
! D49   D(14,16,19,21)       0.0           -DE/DX =    0.0             !
! D50   D(14,16,19,23)      180.0           -DE/DX =    0.0             !
! D51   D(20,16,19,21)      180.0           -DE/DX =    0.0             !
! D52   D(20,16,19,23)       0.0           -DE/DX =    0.0             !
! D53   D(15,17,21,19)       0.0           -DE/DX =    0.0             !
! D54   D(15,17,21,24)      180.0           -DE/DX =    0.0             !
! D55   D(22,17,21,19)      180.0           -DE/DX =    0.0             !
! D56   D(22,17,21,24)       0.0           -DE/DX =    0.0             !
! D57   D(16,19,21,17)       0.0           -DE/DX =    0.0             !
! D58   D(16,19,21,24)      180.0           -DE/DX =    0.0             !
! D59   D(23,19,21,17)      180.0           -DE/DX =    0.0             !
! D60   D(23,19,21,24)       0.0           -DE/DX =    0.0             !
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 ------------------
 - Thermochemistry -
 ------------------
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.

 Zero-point correction=                           0.186929 (Hartree/Particle)
```

Thermal correction to Energy= 0.197746
Thermal correction to Enthalpy= 0.198690
Thermal correction to Gibbs Free Energy= 0.149468
Sum of electronic and zero-point Energies= -637.716190
Sum of electronic and thermal Energies= -637.705373
Sum of electronic and thermal Enthalpies= -637.704429
Sum of electronic and thermal Free Energies= -637.753651

Catechol 3.2C

****
%nprocshared=4
Will use up to 4 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thusini\Reproducing data of li et. al paper\BDOB-Gas phase-7-
16\FREQ-CAT-GAS PHASE.chk
---
freq wb97xd/6-31g(d,p) geom=connectivity

1/10=4,30=1,38=1,57=2/1,3;
2/12=2,17=6,18=5,40=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
4//1;
5/5=2,38=5,98=1/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1/2;
6/7=2,8=2,9=2,10=2,18=1,28=1/1;
7/8=1,10=1,25=1/1,2,3,16;
1/10=4,30=1/3;
99//99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.8753	0.73105	0.00003
C	-0.65034	1.39902	-0.00002
C	0.53061	0.67289	0.00001
C	0.50342	-0.72913	-0.00004
C	-0.71785	-1.38798	-0.00004
C	-1.90557	-0.6578	-0.00001
H	-2.79775	1.30138	0.00003
H	-0.61465	2.4859	0.00004
H	-0.71917	-2.47249	0.

H	-2.8552	-1.18204	0.00003
O	1.66107	-1.43495	0.00007
H	2.38834	-0.80148	-0.00033
O	1.78481	1.22468	0.00005
H	1.72156	2.18258	-0.00028

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Berny optimization.
Initialization pass.
Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run= 2 maximum allowed number of steps= 2.

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- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.110551 (Hartree/Particle)
Thermal correction to Energy= 0.117260
Thermal correction to Enthalpy= 0.118204
Thermal correction to Gibbs Free Energy= 0.080054
Sum of electronic and zero-point Energies= -382.463261
Sum of electronic and thermal Energies= -382.456552
Sum of electronic and thermal Enthalpies= -382.455608
Sum of electronic and thermal Free Energies= -382.493758

GeomOPT INT-C (**3.7C**)

****
%mem=1GB
%chk=T:\CHM\deg013\Thusini\Reproducing data of li et. al paper\BDOB-Gas phase-7-16\BDOB-1st reaction-7-20\BDOB-1st reaction-gas phase-7-20\TPH-01-46-OPT-INT-1-T2-gas phase.chk
---
opt wb97xd/6-31g(d,p) geom=connectivity

1/14=-1,18=20,19=15,26=3,38=1,57=2/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;

4//1;
5/5=2,38=5/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(2);
2/9=110/2;
99//99;
2/9=110/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	1.6981	-0.37737	0.09938
C	2.55823	0.69712	0.36399
C	3.93036	0.54945	0.18505
C	4.45798	-0.66271	-0.24836
C	3.60977	-1.73358	-0.50822
C	2.23847	-1.58564	-0.32997
H	4.58687	1.39075	0.39134
H	5.52936	-0.76357	-0.38212
H	4.01063	-2.68218	-0.84773
H	1.55307	-2.40478	-0.51904
C	-2.08479	0.13371	-0.06269
C	-3.11153	1.01452	-0.4297
C	-2.44255	-1.14222	0.39365
C	-4.44817	0.63755	-0.34509
H	-2.85343	2.00785	-0.78529
C	-3.77695	-1.52613	0.48369
H	-1.66195	-1.83976	0.68298
C	-4.78185	-0.63499	0.11355
H	-5.22937	1.33381	-0.63432
H	-4.03476	-2.51821	0.84188
H	-5.82422	-0.93123	0.18414
O	0.35034	-0.32661	0.30752
B	-0.58619	0.57985	-0.16403
O	-0.28498	1.78909	-0.69914
H	0.60921	2.07909	-0.47098

O	1.99467	1.87306	0.78231
H	2.6828	2.52642	0.94212

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! R23	R(16,20)	1.0859	-DE/DX = 0.0	!
! R24	R(18,21)	1.0861	-DE/DX = 0.0	!
! R25	R(22,23)	1.3883	-DE/DX = -0.0001	!
! R26	R(23,24)	1.3554	-DE/DX = 0.0	!
! R27	R(24,25)	0.9656	-DE/DX = 0.0	!
! R28	R(26,27)	0.9613	-DE/DX = 0.0	!
! A1	A(2,1,6)	118.799	-DE/DX = 0.0	!
! A2	A(2,1,22)	123.4757	-DE/DX = 0.0	!
! A3	A(6,1,22)	117.6336	-DE/DX = 0.0	!
! A4	A(1,2,3)	120.094	-DE/DX = 0.0	!
! A5	A(1,2,26)	117.6754	-DE/DX = 0.0	!
! A6	A(3,2,26)	122.2254	-DE/DX = 0.0	!
! A7	A(2,3,4)	120.4946	-DE/DX = 0.0	!
! A8	A(2,3,7)	119.2958	-DE/DX = 0.0	!
! A9	A(4,3,7)	120.2093	-DE/DX = 0.0	!
! A10	A(3,4,5)	119.7244	-DE/DX = 0.0	!
! A11	A(3,4,8)	119.6915	-DE/DX = 0.0	!
! A12	A(5,4,8)	120.584	-DE/DX = 0.0	!
! A13	A(4,5,6)	119.7576	-DE/DX = 0.0	!
! A14	A(4,5,9)	120.4024	-DE/DX = 0.0	!
! A15	A(6,5,9)	119.8399	-DE/DX = 0.0	!
! A16	A(1,6,5)	121.1284	-DE/DX = 0.0	!
! A17	A(1,6,10)	117.4635	-DE/DX = 0.0	!
! A18	A(5,6,10)	121.408	-DE/DX = 0.0	!
! A19	A(12,11,13)	118.1302	-DE/DX = 0.0	!
! A20	A(12,11,23)	120.2072	-DE/DX = 0.0	!
! A21	A(13,11,23)	121.6624	-DE/DX = 0.0	!
! A22	A(11,12,14)	121.1067	-DE/DX = 0.0	!
! A23	A(11,12,15)	118.9911	-DE/DX = 0.0	!
! A24	A(14,12,15)	119.9022	-DE/DX = 0.0	!
! A25	A(11,13,16)	121.0972	-DE/DX = 0.0	!
! A26	A(11,13,17)	119.1415	-DE/DX = 0.0	!
! A27	A(16,13,17)	119.761	-DE/DX = 0.0	!
! A28	A(12,14,18)	119.8499	-DE/DX = 0.0	!
! A29	A(12,14,19)	120.0855	-DE/DX = 0.0	!
! A30	A(18,14,19)	120.0644	-DE/DX = 0.0	!
! A31	A(13,16,18)	119.8628	-DE/DX = 0.0	!
! A32	A(13,16,20)	120.0865	-DE/DX = 0.0	!
! A33	A(18,16,20)	120.0507	-DE/DX = 0.0	!
! A34	A(14,18,16)	119.9528	-DE/DX = 0.0	!
! A35	A(14,18,21)	120.0237	-DE/DX = 0.0	!
! A36	A(16,18,21)	120.0234	-DE/DX = 0.0	!
! A37	A(1,22,23)	129.9789	-DE/DX = 0.0	!
! A38	A(11,23,22)	115.9929	-DE/DX = 0.0	!
! A39	A(11,23,24)	119.5847	-DE/DX = 0.0	!
! A40	A(22,23,24)	124.4202	-DE/DX = 0.0	!

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! A41   A(23,24,25)        112.5167       -DE/DX =    0.0             !
! A42   A(2,26,27)         109.5429       -DE/DX =    0.0             !
! D1    D(6,1,2,3)          0.4887       -DE/DX =    0.0             !
! D2    D(6,1,2,26)       179.6818       -DE/DX =    0.0             !
! D3    D(22,1,2,3)       176.9199       -DE/DX =    0.0             !
! D4    D(22,1,2,26)       -3.8869       -DE/DX =    0.0             !
! D5    D(2,1,6,5)         -0.4371       -DE/DX =    0.0             !
! D6    D(2,1,6,10)       179.4327       -DE/DX =    0.0             !
! D7    D(22,1,6,5)      -177.0773       -DE/DX =    0.0             !
! D8    D(22,1,6,10)        2.7925       -DE/DX =    0.0             !
! D9    D(2,1,22,23)       54.5731       -DE/DX =    0.0             !
! D10   D(6,1,22,23)     -128.9568       -DE/DX =    0.0             !
! D11   D(1,2,3,4)         -0.397        -DE/DX =    0.0             !
! D12   D(1,2,3,7)        179.789        -DE/DX =    0.0             !
! D13   D(26,2,3,4)       -179.5523       -DE/DX =    0.0            !
! D14   D(26,2,3,7)         0.6336       -DE/DX =    0.0             !
! D15   D(1,2,26,27)      176.4977       -DE/DX =    0.0             !
! D16   D(3,2,26,27)       -4.3276       -DE/DX =    0.0             !
! D17   D(2,3,4,5)          0.2409       -DE/DX =    0.0             !
! D18   D(2,3,4,8)       -179.8942       -DE/DX =    0.0             !
! D19   D(7,3,4,5)       -179.9467       -DE/DX =    0.0             !
! D20   D(7,3,4,8)         -0.0818       -DE/DX =    0.0             !
! D21   D(3,4,5,6)         -0.1831       -DE/DX =    0.0             !
! D22   D(3,4,5,9)        179.8713       -DE/DX =    0.0             !
! D23   D(8,4,5,6)        179.9532       -DE/DX =    0.0             !
! D24   D(8,4,5,9)          0.0076       -DE/DX =    0.0             !
! D25   D(4,5,6,1)          0.2871       -DE/DX =    0.0             !
! D26   D(4,5,6,10)      -179.5775       -DE/DX =    0.0             !
! D27   D(9,5,6,1)       -179.7669       -DE/DX =    0.0             !
! D28   D(9,5,6,10)         0.3684       -DE/DX =    0.0             !
! D29   D(13,11,12,14)     -0.036        -DE/DX =    0.0             !
! D30   D(13,11,12,15)    179.9923       -DE/DX =    0.0             !
! D31   D(23,11,12,14)   -179.8885       -DE/DX =    0.0             !
! D32   D(23,11,12,15)      0.1398       -DE/DX =    0.0             !
! D33   D(12,11,13,16)     -0.1441       -DE/DX =    0.0             !
! D34   D(12,11,13,17)   -179.9385       -DE/DX =    0.0             !
! D35   D(23,11,13,16)    179.7061       -DE/DX =    0.0             !
! D36   D(23,11,13,17)     -0.0883       -DE/DX =    0.0             !
! D37   D(12,11,23,22)    177.2929       -DE/DX =    0.0             !
! D38   D(12,11,23,24)     -3.2244       -DE/DX =    0.0             !
! D39   D(13,11,23,22)     -2.5543       -DE/DX =    0.0             !
! D40   D(13,11,23,24)    176.9284       -DE/DX =    0.0             !
! D41   D(11,12,14,18)      0.1737       -DE/DX =    0.0             !
! D42   D(11,12,14,19)   -179.9481       -DE/DX =    0.0             !
! D43   D(15,12,14,18)   -179.8548       -DE/DX =    0.0             !
! D44   D(15,12,14,19)      0.0234       -DE/DX =    0.0             !
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 ! D45   D(11,13,16,18)        0.1853         -DE/DX =    0.0              !
 ! D46   D(11,13,16,20)     -179.7621          -DE/DX =    0.0              !
 ! D47   D(17,13,16,18)      179.9785          -DE/DX =    0.0              !
 ! D48   D(17,13,16,20)        0.031          -DE/DX =    0.0              !
 ! D49   D(12,14,18,16)       -0.1326         -DE/DX =    0.0              !
 ! D50   D(12,14,18,21)      179.7465          -DE/DX =    0.0              !
 ! D51   D(19,14,18,16)      179.9892          -DE/DX =    0.0              !
 ! D52   D(19,14,18,21)       -0.1317         -DE/DX =    0.0              !
 ! D53   D(13,16,18,14)       -0.0446         -DE/DX =    0.0              !
 ! D54   D(13,16,18,21)     -179.9236          -DE/DX =    0.0              !
 ! D55   D(20,16,18,14)      179.9029          -DE/DX =    0.0              !
 ! D56   D(20,16,18,21)        0.0238         -DE/DX =    0.0              !
 ! D57   D(1,22,23,11)       163.9769          -DE/DX =    0.0              !
 ! D58   D(1,22,23,24)       -15.4779          -DE/DX =    0.0              !
 ! D59   D(11,23,24,25)      162.4129          -DE/DX =    0.0              !
 ! D60   D(22,23,24,25)      -18.1507          -DE/DX =    0.0              !
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```

GradGradGradG

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	1.69519	-0.37615	0.09385
C	2.55932	0.69254	0.36856
C	3.93095	0.54375	0.19123
C	4.45845	-0.6648	-0.25093
C	3.60771	-1.72997	-0.52224
C	2.23688	-1.58038	-0.34597
H	4.58926	1.38261	0.40502
H	5.52989	-0.76693	-0.38304
H	4.00695	-2.67647	-0.86949
H	1.5494	-2.39571	-0.54306
C	-2.0858	0.13421	-0.06216
C	-3.11121	1.00575	-0.45235
C	-2.44263	-1.13251	0.41802
C	-4.44685	0.62741	-0.36758
H	-2.85038	1.99134	-0.82661
C	-3.77627	-1.51673	0.50921
H	-1.66101	-1.82087	0.72596
C	-4.78023	-0.6356	0.11536
H	-5.22811	1.31576	-0.67532
H	-4.03448	-2.50128	0.88747
H	-5.82252	-0.93245	0.18662
O	0.3508	-0.32666	0.30017
B	-0.59	0.5827	-0.16397
O	-0.28903	1.7938	-0.693
H	0.60384	2.08424	-0.46755
O	2.00044	1.8704	0.79413
H	2.69643	2.50087	0.99938

GradGradGradG

Sum of electronic and thermal Energies= -714.086881
Sum of electronic and thermal Enthalpies= -714.085937
Sum of electronic and thermal Free Energies= -714.141815

BDOB-W1 (**3.4C**)

****
%nprocshared=2
Will use up to 2 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thusini\Reproducing data of li et. al paper\BDOB-Gas phase-7-
16\BDOB-1st reaction-7-20\BDOB-1st reaction-gas phase-7-20\TPH-01-46-OPT-BDOB-W1
-gas phase.chk
---
opt wb97xd/6-31g(d,p) geom=connectivity

1/14=-1,18=20,19=15,26=3,38=1,57=2/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4//1;
5/5=2,38=5/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(2);
2/9=110/2;
99//99;
2/9=110/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1
C -1.87818 0.65491 0.2626
C -1.87336 -0.72615 0.08917
C -3.03965 -1.45935 0.01193
C -4.23632 -0.74243 0.11974

C	-4.2417	0.64173	0.29513
C	-3.05143	1.37336	0.36952
H	-3.02305	-2.53416	-0.12583
H	-5.17913	-1.27598	0.06563
H	-5.18885	1.16388	0.37729
H	-3.04411	2.44815	0.5071
B	0.20179	-0.02355	0.17862
O	-0.58647	1.11149	0.29694
O	-0.57605	-1.16691	0.0141
C	1.74907	-0.0233	0.14702
C	2.46118	-1.21459	-0.05435
C	2.47195	1.16217	0.34161
C	3.85209	-1.22219	-0.06408
H	1.91854	-2.14322	-0.20771
C	3.8628	1.15916	0.33224
H	1.93769	2.09415	0.50145
C	4.5532	-0.03391	0.12937
H	4.38889	-2.15205	-0.22261
H	4.40819	2.08522	0.4833
H	5.63885	-0.03767	0.1219
O	0.21441	-0.49664	2.08062
H	1.16443	-0.39653	1.96497
H	0.02262	-1.34979	1.67942

Add virtual bond connecting atoms H27 and O13 Dist= 3.36D+00.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.

Item	Value	Threshold	Converged?
Maximum Force	0.000016	0.000450	YES
RMS Force	0.000003	0.000300	YES
Maximum Displacement	0.001146	0.001800	YES
RMS Displacement	0.000284	0.001200	YES

Predicted change in Energy=-7.298925D-09
Optimization completed.
-- Stationary point found.

Optimized Parameters
(Angstroms and Degrees)

Name	Definition	Value	Derivative Info.
R1	R(1,2)	1.3917	-DE/DX = 0.0

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! R2    R(1,6)              1.3795       -DE/DX =    0.0             !
! R3    R(1,12)              1.3699       -DE/DX =    0.0             !
! R4    R(2,3)              1.3794       -DE/DX =    0.0             !
! R5    R(2,13)              1.3725       -DE/DX =    0.0             !
! R6    R(3,4)              1.3986       -DE/DX =    0.0             !
! R7    R(3,7)              1.0837       -DE/DX =    0.0             !
! R8    R(4,5)              1.3947       -DE/DX =    0.0             !
! R9    R(4,8)              1.0847       -DE/DX =    0.0             !
! R10   R(5,6)               1.3985       -DE/DX =    0.0             !
! R11   R(5,9)               1.0847       -DE/DX =    0.0             !
! R12   R(6,10)              1.0835       -DE/DX =    0.0             !
! R13   R(11,12)              1.3848       -DE/DX =    0.0             !
! R14   R(11,13)              1.3926       -DE/DX =    0.0             !
! R15   R(11,14)              1.5484       -DE/DX =    0.0             !
! R16   R(13,27)              2.543        -DE/DX =    0.0             !
! R17   R(14,15)              1.4021       -DE/DX =    0.0             !
! R18   R(14,16)              1.4017       -DE/DX =    0.0             !
! R19   R(15,17)              1.3907       -DE/DX =    0.0             !
! R20   R(15,18)              1.0866       -DE/DX =    0.0             !
! R21   R(16,19)              1.3906       -DE/DX =    0.0             !
! R22   R(16,20)              1.086        -DE/DX =    0.0             !
! R23   R(17,21)              1.3928       -DE/DX =    0.0             !
! R24   R(17,22)              1.0854       -DE/DX =    0.0             !
! R25   R(19,21)              1.3928       -DE/DX =    0.0             !
! R26   R(19,23)              1.0854       -DE/DX =    0.0             !
! R27   R(21,24)              1.0857       -DE/DX =    0.0             !
! R28   R(25,26)              0.962        -DE/DX =    0.0             !
! R29   R(25,27)              0.9616       -DE/DX =    0.0             !
! A1    A(2,1,6)             121.9082       -DE/DX =    0.0             !
! A2    A(2,1,12)            109.3202       -DE/DX =    0.0             !
! A3    A(6,1,12)            128.7707       -DE/DX =    0.0             !
! A4    A(1,2,3)             122.0985       -DE/DX =    0.0             !
! A5    A(1,2,13)            109.1823       -DE/DX =    0.0             !
! A6    A(3,2,13)            128.7188       -DE/DX =    0.0             !
! A7    A(2,3,4)             116.5285       -DE/DX =    0.0             !
! A8    A(2,3,7)             121.3497       -DE/DX =    0.0             !
! A9    A(4,3,7)             122.1218       -DE/DX =    0.0             !
! A10   A(3,4,5)              121.4014       -DE/DX =    0.0             !
! A11   A(3,4,8)              119.1988       -DE/DX =    0.0             !
! A12   A(5,4,8)              119.3998       -DE/DX =    0.0             !
! A13   A(4,5,6)              121.4831       -DE/DX =    0.0             !
! A14   A(4,5,9)              119.3539       -DE/DX =    0.0             !
! A15   A(6,5,9)              119.1629       -DE/DX =    0.0             !
! A16   A(1,6,5)              116.5799       -DE/DX =    0.0             !
! A17   A(1,6,10)             121.2656       -DE/DX =    0.0             !
! A18   A(5,6,10)             122.154        -DE/DX =    0.0             !
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! A19   A(12,11,13)        111.5101       -DE/DX =    0.0             !
! A20   A(12,11,14)        124.8486       -DE/DX =    0.0             !
! A21   A(13,11,14)        123.5611       -DE/DX =    0.0             !
! A22   A(1,12,11)         105.0911       -DE/DX =    0.0             !
! A23   A(2,13,11)         104.8363       -DE/DX =    0.0             !
! A24   A(2,13,27)         104.4129       -DE/DX =    0.0             !
! A25   A(11,13,27)         82.6903       -DE/DX =    0.0             !
! A26   A(11,14,15)        120.6877       -DE/DX =    0.0             !
! A27   A(11,14,16)        120.8444       -DE/DX =    0.0             !
! A28   A(15,14,16)        118.4506       -DE/DX =    0.0             !
! A29   A(14,15,17)        120.8947       -DE/DX =    0.0             !
! A30   A(14,15,18)        119.4186       -DE/DX =    0.0             !
! A31   A(17,15,18)        119.686        -DE/DX =    0.0             !
! A32   A(14,16,19)        120.8309       -DE/DX =    0.0             !
! A33   A(14,16,20)        119.3596       -DE/DX =    0.0             !
! A34   A(19,16,20)        119.8095       -DE/DX =    0.0             !
! A35   A(15,17,21)        119.8374       -DE/DX =    0.0             !
! A36   A(15,17,22)        120.033        -DE/DX =    0.0             !
! A37   A(21,17,22)        120.1296       -DE/DX =    0.0             !
! A38   A(16,19,21)        119.9122       -DE/DX =    0.0             !
! A39   A(16,19,23)        119.9784       -DE/DX =    0.0             !
! A40   A(21,19,23)        120.1095       -DE/DX =    0.0             !
! A41   A(17,21,19)        120.0742       -DE/DX =    0.0             !
! A42   A(17,21,24)        119.9542       -DE/DX =    0.0             !
! A43   A(19,21,24)        119.9716       -DE/DX =    0.0             !
! A44   A(26,25,27)        103.9389       -DE/DX =    0.0             !
! A45   A(13,27,25)        110.7814       -DE/DX =    0.0             !
! D1    D(6,1,2,3)           0.1605       -DE/DX =    0.0             !
! D2    D(6,1,2,13)        179.9661       -DE/DX =    0.0             !
! D3    D(12,1,2,3)       -179.5445       -DE/DX =    0.0             !
! D4    D(12,1,2,13)         0.2611       -DE/DX =    0.0             !
! D5    D(2,1,6,5)          -0.0063       -DE/DX =    0.0             !
! D6    D(2,1,6,10)        179.7337       -DE/DX =    0.0             !
! D7    D(12,1,6,5)        179.6366       -DE/DX =    0.0             !
! D8    D(12,1,6,10)        -0.6234       -DE/DX =    0.0             !
! D9    D(2,1,12,11)        -1.6551       -DE/DX =    0.0             !
! D10   D(6,1,12,11)       178.6662       -DE/DX =    0.0             !
! D11   D(1,2,3,4)          -0.1806       -DE/DX =    0.0             !
! D12   D(1,2,3,7)         179.7271       -DE/DX =    0.0             !
! D13   D(13,2,3,4)       -179.9453       -DE/DX =    0.0             !
! D14   D(13,2,3,7)         -0.0375       -DE/DX =    0.0             !
! D15   D(1,2,13,11)         1.2412       -DE/DX =    0.0             !
! D16   D(1,2,13,27)        87.3522       -DE/DX =    0.0             !
! D17   D(3,2,13,11)      -178.9699       -DE/DX =    0.0             !
! D18   D(3,2,13,27)        -92.8589       -DE/DX =    0.0             !
! D19   D(2,3,4,5)           0.0572       -DE/DX =    0.0             !
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! D20   D(2,3,4,8)         -179.9259       -DE/DX =    0.0             !
! D21   D(7,3,4,5)         -179.8498       -DE/DX =    0.0             !
! D22   D(7,3,4,8)           0.1671       -DE/DX =    0.0             !
! D23   D(3,4,5,6)           0.092        -DE/DX =    0.0             !
! D24   D(3,4,5,9)         -179.8101       -DE/DX =    0.0             !
! D25   D(8,4,5,6)         -179.9249       -DE/DX =    0.0             !
! D26   D(8,4,5,9)           0.1729       -DE/DX =    0.0             !
! D27   D(4,5,6,1)           -0.1159       -DE/DX =    0.0             !
! D28   D(4,5,6,10)        -179.8534       -DE/DX =    0.0             !
! D29   D(9,5,6,1)          179.7864       -DE/DX =    0.0             !
! D30   D(9,5,6,10)          0.0489       -DE/DX =    0.0             !
! D31   D(13,11,12,1)        2.5085       -DE/DX =    0.0             !
! D32   D(14,11,12,1)      179.342        -DE/DX =    0.0             !
! D33   D(12,11,13,2)       -2.3504       -DE/DX =    0.0             !
! D34   D(12,11,13,27)    -105.3899       -DE/DX =    0.0             !
! D35   D(14,11,13,2)     -179.2319       -DE/DX =    0.0             !
! D36   D(14,11,13,27)      77.7285       -DE/DX =    0.0             !
! D37   D(12,11,14,15)    -174.5469       -DE/DX =    0.0             !
! D38   D(12,11,14,16)       6.9866       -DE/DX =    0.0             !
! D39   D(13,11,14,15)       1.9174       -DE/DX =    0.0             !
! D40   D(13,11,14,16)    -176.5492       -DE/DX =    0.0             !
! D41   D(2,13,27,25)      -77.4329       -DE/DX =    0.0             !
! D42   D(11,13,27,25)      26.0749       -DE/DX =    0.0             !
! D43   D(11,14,15,17)    -178.6164       -DE/DX =    0.0             !
! D44   D(11,14,15,18)       1.6996       -DE/DX =    0.0             !
! D45   D(16,14,15,17)      -0.1138       -DE/DX =    0.0             !
! D46   D(16,14,15,18)    -179.7978       -DE/DX =    0.0             !
! D47   D(11,14,16,19)     178.6022       -DE/DX =    0.0             !
! D48   D(11,14,16,20)      -1.3402       -DE/DX =    0.0             !
! D49   D(15,14,16,19)       0.1021       -DE/DX =    0.0             !
! D50   D(15,14,16,20)    -179.8404       -DE/DX =    0.0             !
! D51   D(14,15,17,21)       0.0863       -DE/DX =    0.0             !
! D52   D(14,15,17,22)    -179.8702       -DE/DX =    0.0             !
! D53   D(18,15,17,21)     179.7695       -DE/DX =    0.0             !
! D54   D(18,15,17,22)      -0.1871       -DE/DX =    0.0             !
! D55   D(14,16,19,21)      -0.063        -DE/DX =    0.0             !
! D56   D(14,16,19,23)     179.9659       -DE/DX =    0.0             !
! D57   D(20,16,19,21)     179.8792       -DE/DX =    0.0             !
! D58   D(20,16,19,23)      -0.0919       -DE/DX =    0.0             !
! D59   D(15,17,21,19)      -0.0447       -DE/DX =    0.0             !
! D60   D(15,17,21,24)     179.9674       -DE/DX =    0.0             !
! D61   D(22,17,21,19)     179.9118       -DE/DX =    0.0             !
! D62   D(22,17,21,24)      -0.0761       -DE/DX =    0.0             !
! D63   D(16,19,21,17)       0.0332       -DE/DX =    0.0             !
! D64   D(16,19,21,24)    -179.9789       -DE/DX =    0.0             !
! D65   D(23,19,21,17)    -179.9958       -DE/DX =    0.0             !
```

```
 ! D66   D(23,19,21,24)        -0.0079         -DE/DX =    0.0              !
 ! D67   D(26,25,27,13)        -88.8132        -DE/DX =    0.0              !
 ---------------------------------------------------------------------------
```

GradGradGradG

O	-0.59842	1.21466	-0.12871
O	-0.58364	-1.06871	-0.36816
C	1.73814	0.08017	-0.26655
C	2.44826	-1.10889	-0.48523
C	2.46262	1.26049	-0.0502
C	3.8389	-1.11948	-0.49029
H	1.90247	-2.03242	-0.65792
C	3.85322	1.25407	-0.05425
H	1.92753	2.18946	0.12332
C	4.54167	0.06338	-0.27407
H	4.37447	-2.0476	-0.6631
H	4.4003	2.17619	0.11425
H	5.62739	0.0572	-0.27709
O	0.296	-0.58783	2.48177
H	1.23195	-0.45262	2.30549
H	0.0988	-1.42684	2.05529

GradGradGradG

%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\Method validatio
n\TPH-01-46-Gas phase- using file-FREQ-INT1-W2-BDOB.chk
---
opt freq wb97xd/6-31g(d,p)

1/14=-1,18=20,19=15,26=3,38=1/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4//1;
5/5=2,38=5/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(2);
2/9=110/2;
99//99;
2/9=110/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.76633	-0.2716	-0.42073
C	-2.50022	0.88683	-0.14171
C	-3.88368	0.81465	-0.01553
C	-4.5361	-0.40674	-0.16554
C	-3.80788	-1.55706	-0.44618
C	-2.42299	-1.4845	-0.57504
H	-4.44919	1.71661	0.20307
H	-5.61483	-0.4519	-0.06144
H	-4.31051	-2.51047	-0.56543
H	-1.83356	-2.36822	-0.79335
B	0.49831	-0.65744	0.31729
O	-0.41289	-0.1593	-0.58883
C	2.0136	-0.40248	-0.0141
C	2.37235	0.54874	-0.98117
C	3.04457	-1.09302	0.63581

C	3.70659	0.8101	-1.27656
H	1.58784	1.08778	-1.505
C	4.38146	-0.84352	0.34189
H	2.81161	-1.85181	1.37971
C	4.71425	0.11311	-0.61369
H	3.9622	1.55371	-2.02486
H	5.16328	-1.39298	0.85676
H	5.75657	0.31264	-0.84201
O	-1.80184	2.05451	-0.01156
H	-2.40452	2.76463	0.23022
O	0.0398	-1.38264	1.37222
H	0.72109	-1.58994	2.01475
O	0.561	1.90979	1.65622
H	1.32808	1.94794	1.07755
H	-0.19193	2.00325	1.05443

Add virtual bond connecting atoms H30 and O24 Dist= 3.65D+00.

GradGradGradG

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! R9    R(4,8)              1.0847        -DE/DX =    0.0              !
! R10   R(5,6)              1.3923        -DE/DX =    0.0              !
! R11   R(5,9)              1.0844        -DE/DX =    0.0              !
! R12   R(6,10)             1.0843        -DE/DX =    0.0              !
! R13   R(11,12)            1.3785        -DE/DX =    0.0              !
! R14   R(11,13)            1.5726        -DE/DX =    0.0              !
! R15   R(11,26)            1.3598        -DE/DX =    0.0              !
! R16   R(13,14)            1.4024        -DE/DX =    0.0              !
! R17   R(13,15)            1.3998        -DE/DX =    0.0              !
! R18   R(14,16)            1.3909        -DE/DX =    0.0              !
! R19   R(14,17)            1.0866        -DE/DX =    0.0              !
! R20   R(15,18)            1.3911        -DE/DX =    0.0              !
! R21   R(15,19)            1.0882        -DE/DX =    0.0              !
! R22   R(16,20)            1.3928        -DE/DX =    0.0              !
! R23   R(16,21)            1.0856        -DE/DX =    0.0              !
! R24   R(18,20)            1.3919        -DE/DX =    0.0              !
! R25   R(18,22)            1.0856        -DE/DX =    0.0              !
! R26   R(20,23)            1.0856        -DE/DX =    0.0              !
! R27   R(24,25)            0.9613        -DE/DX =    0.0              !
! R28   R(24,30)            1.9414        -DE/DX =    0.0              !
! R29   R(26,27)            0.9585        -DE/DX =    0.0              !
! R30   R(28,29)            0.9613        -DE/DX =    0.0              !
! R31   R(28,30)            0.9677        -DE/DX =    0.0              !
! A1    A(2,1,6)           119.6696       -DE/DX =    0.0              !
! A2    A(2,1,12)          118.6281       -DE/DX =    0.0              !
! A3    A(6,1,12)          121.6508       -DE/DX =    0.0              !
! A4    A(1,2,3)           119.882        -DE/DX =    0.0              !
! A5    A(1,2,24)          117.3624       -DE/DX =    0.0              !
! A6    A(3,2,24)          122.7553       -DE/DX =    0.0              !
! A7    A(2,3,4)           120.1425       -DE/DX =    0.0              !
! A8    A(2,3,7)           119.5441       -DE/DX =    0.0              !
! A9    A(4,3,7)           120.313        -DE/DX =    0.0              !
! A10   A(3,4,5)           120.028        -DE/DX =    0.0              !
! A11   A(3,4,8)           119.5329       -DE/DX =    0.0              !
! A12   A(5,4,8)           120.4391       -DE/DX =    0.0              !
! A13   A(4,5,6)           119.8051       -DE/DX =    0.0              !
! A14   A(4,5,9)           120.4266       -DE/DX =    0.0              !
! A15   A(6,5,9)           119.7682       -DE/DX =    0.0              !
! A16   A(1,6,5)           120.4723       -DE/DX =    0.0              !
! A17   A(1,6,10)          118.3486       -DE/DX =    0.0              !
! A18   A(5,6,10)          121.1783       -DE/DX =    0.0              !
! A19   A(12,11,13)        116.0352       -DE/DX =    0.0              !
! A20   A(12,11,26)        118.7449       -DE/DX =    0.0              !
! A21   A(13,11,26)        125.0221       -DE/DX =    0.0              !
! A22   A(1,12,11)         122.6632       -DE/DX =    0.0              !
! A23   A(11,13,14)        120.2484       -DE/DX =    0.0              !
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! A24   A(11,13,15)          121.9782        -DE/DX =    0.0             !
! A25   A(14,13,15)          117.7709        -DE/DX =    0.0             !
! A26   A(13,14,16)          121.228         -DE/DX =    0.0             !
! A27   A(13,14,17)          118.8219        -DE/DX =    0.0             !
! A28   A(16,14,17)          119.95          -DE/DX =    0.0             !
! A29   A(13,15,18)          121.4196        -DE/DX =    0.0             !
! A30   A(13,15,19)          120.0198        -DE/DX =    0.0             !
! A31   A(18,15,19)          118.555         -DE/DX =    0.0             !
! A32   A(14,16,20)          119.936         -DE/DX =    0.0             !
! A33   A(14,16,21)          120.0693        -DE/DX =    0.0             !
! A34   A(20,16,21)          119.9943        -DE/DX =    0.0             !
! A35   A(15,18,20)          119.8238        -DE/DX =    0.0             !
! A36   A(15,18,22)          120.1078        -DE/DX =    0.0             !
! A37   A(20,18,22)          120.0684        -DE/DX =    0.0             !
! A38   A(16,20,18)          119.8167        -DE/DX =    0.0             !
! A39   A(16,20,23)          120.168         -DE/DX =    0.0             !
! A40   A(18,20,23)          120.0151        -DE/DX =    0.0             !
! A41   A(2,24,25)           109.0982        -DE/DX =    0.0             !
! A42   A(2,24,30)           116.2235        -DE/DX =    0.0             !
! A43   A(25,24,30)          113.9125        -DE/DX =    0.0             !
! A44   A(11,26,27)          112.5572        -DE/DX =    0.0             !
! A45   A(29,28,30)          104.2421        -DE/DX =    0.0             !
! A46   L(24,30,28,11,-1)    176.2086        -DE/DX =    0.0             !
! A47   L(24,30,28,11,-2)    185.2627        -DE/DX =    0.0             !
! D1    D(6,1,2,3)           -0.0314         -DE/DX =    0.0             !
! D2    D(6,1,2,24)          -179.8427       -DE/DX =    0.0             !
! D3    D(12,1,2,3)          177.4014        -DE/DX =    0.0             !
! D4    D(12,1,2,24)         -2.4099         -DE/DX =    0.0             !
! D5    D(2,1,6,5)           -0.1394         -DE/DX =    0.0             !
! D6    D(2,1,6,10)          -179.8251       -DE/DX =    0.0             !
! D7    D(12,1,6,5)          -177.4922       -DE/DX =    0.0             !
! D8    D(12,1,6,10)         2.822           -DE/DX =    0.0             !
! D9    D(2,1,12,11)         107.0809        -DE/DX =    0.0             !
! D10   D(6,1,12,11)         -75.5395        -DE/DX =    0.0             !
! D11   D(1,2,3,4)           0.1837          -DE/DX =    0.0             !
! D12   D(1,2,3,7)           179.9726        -DE/DX =    0.0             !
! D13   D(24,2,3,4)          179.9845        -DE/DX =    0.0             !
! D14   D(24,2,3,7)          -0.2266         -DE/DX =    0.0             !
! D15   D(1,2,24,25)         -176.164        -DE/DX =    0.0             !
! D16   D(1,2,24,30)         -45.7192        -DE/DX =    0.0             !
! D17   D(3,2,24,25)         4.0305          -DE/DX =    0.0             !
! D18   D(3,2,24,30)         134.4753        -DE/DX =    0.0             !
! D19   D(2,3,4,5)           -0.1661         -DE/DX =    0.0             !
! D20   D(2,3,4,8)           179.7551        -DE/DX =    0.0             !
! D21   D(7,3,4,5)           -179.9533       -DE/DX =    0.0             !
! D22   D(7,3,4,8)           -0.0321         -DE/DX =    0.0             !
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 ! D23   D(3,4,5,6)          -0.0042        -DE/DX =    0.0             !
 ! D24   D(3,4,5,9)          179.9298        -DE/DX =    0.0             !
 ! D25   D(8,4,5,6)         -179.9247        -DE/DX =    0.0             !
 ! D26   D(8,4,5,9)           0.0093        -DE/DX =    0.0             !
 ! D27   D(4,5,6,1)           0.1575        -DE/DX =    0.0             !
 ! D28   D(4,5,6,10)          179.8342        -DE/DX =    0.0             !
 ! D29   D(9,5,6,1)         -179.777         -DE/DX =    0.0             !
 ! D30   D(9,5,6,10)          -0.1002        -DE/DX =    0.0             !
 ! D31   D(13,11,12,1)      -177.9661         -DE/DX =    0.0             !
 ! D32   D(26,11,12,1)         6.8858        -DE/DX =    0.0             !
 ! D33   D(12,11,13,14)       16.6894         -DE/DX =    0.0             !
 ! D34   D(12,11,13,15)     -163.8973         -DE/DX =    0.0             !
 ! D35   D(26,11,13,14)     -168.5061         -DE/DX =    0.0             !
 ! D36   D(26,11,13,15)       10.9072         -DE/DX =    0.0             !
 ! D37   D(12,11,26,27)     -167.1686         -DE/DX =    0.0             !
 ! D38   D(13,11,26,27)       18.1562         -DE/DX =    0.0             !
 ! D39   D(11,13,14,16)      178.6245         -DE/DX =    0.0             !
 ! D40   D(11,13,14,17)       -1.5106         -DE/DX =    0.0             !
 ! D41   D(15,13,14,16)       -0.8131         -DE/DX =    0.0             !
 ! D42   D(15,13,14,17)      179.0517         -DE/DX =    0.0             !
 ! D43   D(11,13,15,18)     -178.9638         -DE/DX =    0.0             !
 ! D44   D(11,13,15,19)        1.9077        -DE/DX =    0.0             !
 ! D45   D(14,13,15,18)        0.4635        -DE/DX =    0.0             !
 ! D46   D(14,13,15,19)     -178.665         -DE/DX =    0.0             !
 ! D47   D(13,14,16,20)        0.5423        -DE/DX =    0.0             !
 ! D48   D(13,14,16,21)     -179.6951         -DE/DX =    0.0             !
 ! D49   D(17,14,16,20)     -179.3211         -DE/DX =    0.0             !
 ! D50   D(17,14,16,21)        0.4416        -DE/DX =    0.0             !
 ! D51   D(13,15,18,20)        0.1565        -DE/DX =    0.0             !
 ! D52   D(13,15,18,22)     -179.8356         -DE/DX =    0.0             !
 ! D53   D(19,15,18,20)      179.2973         -DE/DX =    0.0             !
 ! D54   D(19,15,18,22)       -0.6947         -DE/DX =    0.0             !
 ! D55   D(14,16,20,18)        0.1009        -DE/DX =    0.0             !
 ! D56   D(14,16,20,23)      179.9228         -DE/DX =    0.0             !
 ! D57   D(21,16,20,18)     -179.6619         -DE/DX =    0.0             !
 ! D58   D(21,16,20,23)        0.16          -DE/DX =    0.0             !
 ! D59   D(15,18,20,16)       -0.4449         -DE/DX =    0.0             !
 ! D60   D(15,18,20,23)      179.733          -DE/DX =    0.0             !
 ! D61   D(22,18,20,16)      179.5472         -DE/DX =    0.0             !
 ! D62   D(22,18,20,23)       -0.275         -DE/DX =    0.0             !
 ! D63   D(2,24,28,29)       112.9578         -DE/DX =    0.0             !
 ! D64   D(25,24,28,29)     -120.163          -DE/DX =    0.0             !
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GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradG
radGrad
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- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.238097 (Hartree/Particle)
Thermal correction to Energy= 0.254649
Thermal correction to Enthalpy= 0.255593
Thermal correction to Gibbs Free Energy= 0.192650
Sum of electronic and zero-point Energies= -790.486672
Sum of electronic and thermal Energies= -790.470120
Sum of electronic and thermal Enthalpies= -790.469176
Sum of electronic and thermal Free Energies= -790.532119

Bound product-BDOB-C 3.2C+3.3

****
%mem=1GB
%nprocshared=4
Will use up to 4 processors via shared memory.
%chk=T:\CHM\deg013\Thusini\Reproducing data of li et. al paper\Heteroborole-7-14
---
opt wb97xd/6-31g(d,p) geom=connectivity

1/14=-1,18=20,19=15,26=3,38=1,57=2/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4//1;
5/5=2,38=5/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(2);
2/9=110/2;
99//99;
2/9=110/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.46813	-0.86262	-0.02453
C	-2.37676	-0.68786	-1.0773
C	-1.63748	-0.07942	1.12596
H	-2.28329	-1.28691	-1.98065
C	-3.41835	0.23012	-0.98597
C	-2.66902	0.84787	1.22089
H	-0.92977	-0.16686	1.94715
C	-3.56343	1.00129	0.16459
H	-4.11686	0.34403	-1.80887
H	-2.77324	1.45343	2.1155
H	-4.37033	1.72387	0.23582
B	-0.2786	-1.88247	-0.12167
O	0.25185	-2.52687	0.95554
O	0.34565	-2.18292	-1.31425
C	0.94798	2.62988	-0.21481
C	1.3515	2.12474	-1.44816
C	1.96685	0.87607	-1.51709
C	2.16142	0.13514	-0.35868
C	1.73192	0.63512	0.87779
C	1.1384	1.89115	0.94964
H	0.47235	3.60324	-0.15536
H	1.19593	2.70017	-2.35432
H	2.30602	0.46646	-2.46375
H	0.80706	2.26242	1.91345
O	2.76741	-1.1003	-0.34665
O	1.86766	-0.12548	1.99173
H	0.03922	-1.62479	-2.03374
H	-0.21639	-2.33619	1.77143
H	2.22044	-0.97687	1.68985
H	2.19205	-1.71388	-0.83308

Add virtual bond connecting atoms H30 and O14 Dist= 3.71D+00.

GradGradGradG

RMS Displacement 0.000210 0.001200 YES
Predicted change in Energy=-1.860917D-08
Optimization completed.
-- Stationary point found.

Optimized Parameters
(Angstroms and Degrees)

Name	Definition	Value	Derivative Info.
R1	R(1,2)	1.4009	-DE/DX = 0.0
R2	R(1,3)	1.4017	-DE/DX = 0.0
R3	R(1,12)	1.5702	-DE/DX = 0.0
R4	R(2,4)	1.0882	-DE/DX = 0.0
R5	R(2,5)	1.391	-DE/DX = 0.0
R6	R(3,6)	1.3898	-DE/DX = 0.0
R7	R(3,7)	1.088	-DE/DX = 0.0
R8	R(5,8)	1.392	-DE/DX = 0.0
R9	R(5,9)	1.0854	-DE/DX = 0.0
R10	R(6,8)	1.3923	-DE/DX = 0.0
R11	R(6,10)	1.0854	-DE/DX = 0.0
R12	R(8,11)	1.0856	-DE/DX = 0.0
R13	R(12,13)	1.362	-DE/DX = 0.0
R14	R(12,14)	1.3788	-DE/DX = 0.0
R15	R(13,28)	0.9593	-DE/DX = 0.0
R16	R(14,27)	0.9605	-DE/DX = 0.0
R17	R(14,30)	1.9895	-DE/DX = 0.0
R18	R(15,16)	1.3922	-DE/DX = 0.0
R19	R(15,20)	1.3915	-DE/DX = 0.0
R20	R(15,21)	1.085	-DE/DX = 0.0
R21	R(16,17)	1.3936	-DE/DX = 0.0
R22	R(16,22)	1.0848	-DE/DX = 0.0
R23	R(17,18)	1.3886	-DE/DX = 0.0
R24	R(17,23)	1.0859	-DE/DX = 0.0
R25	R(18,19)	1.4009	-DE/DX = 0.0
R26	R(18,25)	1.3762	-DE/DX = 0.0
R27	R(19,20)	1.3906	-DE/DX = 0.0
R28	R(19,26)	1.3557	-DE/DX = 0.0
R29	R(20,24)	1.0844	-DE/DX = 0.0
R30	R(25,30)	0.9708	-DE/DX = 0.0
R31	R(26,29)	0.9699	-DE/DX = 0.0
A1	A(2,1,3)	117.9841	-DE/DX = 0.0
A2	A(2,1,12)	121.519	-DE/DX = 0.0
A3	A(3,1,12)	120.4906	-DE/DX = 0.0
A4	A(1,2,4)	119.8404	-DE/DX = 0.0
A5	A(1,2,5)	121.2261	-DE/DX = 0.0

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! A6    A(4,2,5)          118.9269        -DE/DX =    0.0             !
! A7    A(1,3,6)          121.135         -DE/DX =    0.0             !
! A8    A(1,3,7)          119.6182        -DE/DX =    0.0             !
! A9    A(6,3,7)          119.1862        -DE/DX =    0.0             !
! A10   A(2,5,8)           119.798        -DE/DX =    0.0             !
! A11   A(2,5,9)           120.1132        -DE/DX =    0.0             !
! A12   A(8,5,9)           120.0888        -DE/DX =    0.0             !
! A13   A(3,6,8)           119.9169        -DE/DX =    0.0             !
! A14   A(3,6,10)           119.9738        -DE/DX =    0.0             !
! A15   A(8,6,10)           120.1086        -DE/DX =    0.0             !
! A16   A(5,8,6)           119.9376        -DE/DX =    0.0             !
! A17   A(5,8,11)           119.993         -DE/DX =    0.0             !
! A18   A(6,8,11)           120.0688        -DE/DX =    0.0             !
! A19   A(1,12,13)          123.507         -DE/DX =    0.0             !
! A20   A(1,12,14)          122.2176        -DE/DX =    0.0             !
! A21   A(13,12,14)         114.2659        -DE/DX =    0.0             !
! A22   A(12,13,28)         112.2801        -DE/DX =    0.0             !
! A23   A(12,14,27)         111.243         -DE/DX =    0.0             !
! A24   A(12,14,30)          99.3163        -DE/DX =    0.0             !
! A25   A(27,14,30)         109.4687        -DE/DX =    0.0             !
! A26   A(16,15,20)         120.6293        -DE/DX =    0.0             !
! A27   A(16,15,21)         120.0172        -DE/DX =    0.0             !
! A28   A(20,15,21)         119.3523        -DE/DX =    0.0             !
! A29   A(15,16,17)         119.7781        -DE/DX =    0.0             !
! A30   A(15,16,22)         120.3235        -DE/DX =    0.0             !
! A31   A(17,16,22)         119.8956        -DE/DX =    0.0             !
! A32   A(16,17,18)         119.8688        -DE/DX =    0.0             !
! A33   A(16,17,23)         121.3642        -DE/DX =    0.0             !
! A34   A(18,17,23)         118.765         -DE/DX =    0.0             !
! A35   A(17,18,19)         120.2008        -DE/DX =    0.0             !
! A36   A(17,18,25)         123.2417        -DE/DX =    0.0             !
! A37   A(19,18,25)         116.5575        -DE/DX =    0.0             !
! A38   A(18,19,20)         119.9299        -DE/DX =    0.0             !
! A39   A(18,19,26)         119.4418        -DE/DX =    0.0             !
! A40   A(20,19,26)         120.5996        -DE/DX =    0.0             !
! A41   A(15,20,19)         119.5812        -DE/DX =    0.0             !
! A42   A(15,20,24)         121.4062        -DE/DX =    0.0             !
! A43   A(19,20,24)         118.9938        -DE/DX =    0.0             !
! A44   A(18,25,30)         107.4592        -DE/DX =    0.0             !
! A45   A(19,26,29)         105.561         -DE/DX =    0.0             !
! A46   A(14,30,25)         144.1824        -DE/DX =    0.0             !
! D1    D(3,1,2,4)         -179.2584        -DE/DX =    0.0             !
! D2    D(3,1,2,5)           -0.2029        -DE/DX =    0.0             !
! D3    D(12,1,2,4)           1.646         -DE/DX =    0.0             !
! D4    D(12,1,2,5)        -179.2985        -DE/DX =    0.0             !
! D5    D(2,1,3,6)           -0.2498        -DE/DX =    0.0             !
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! D6    D(2,1,3,7)         -177.3937        -DE/DX =    0.0             !
! D7    D(12,1,3,6)         178.8555        -DE/DX =    0.0             !
! D8    D(12,1,3,7)           1.7116        -DE/DX =    0.0             !
! D9    D(2,1,12,13)       -148.2219        -DE/DX =    0.0             !
! D10   D(2,1,12,14)         32.9616        -DE/DX =    0.0             !
! D11   D(3,1,12,13)         32.7049        -DE/DX =    0.0             !
! D12   D(3,1,12,14)       -146.1115        -DE/DX =    0.0             !
! D13   D(1,2,5,8)            0.4078        -DE/DX =    0.0             !
! D14   D(1,2,5,9)         -179.5847        -DE/DX =    0.0             !
! D15   D(4,2,5,8)          179.4718        -DE/DX =    0.0             !
! D16   D(4,2,5,9)           -0.5207        -DE/DX =    0.0             !
! D17   D(1,3,6,8)            0.4951        -DE/DX =    0.0             !
! D18   D(1,3,6,10)        -179.1876        -DE/DX =    0.0             !
! D19   D(7,3,6,8)          177.6511        -DE/DX =    0.0             !
! D20   D(7,3,6,10)          -2.0316        -DE/DX =    0.0             !
! D21   D(2,5,8,6)           -0.1597        -DE/DX =    0.0             !
! D22   D(2,5,8,11)         179.5501        -DE/DX =    0.0             !
! D23   D(9,5,8,6)          179.8328        -DE/DX =    0.0             !
! D24   D(9,5,8,11)          -0.4574        -DE/DX =    0.0             !
! D25   D(3,6,8,5)           -0.2855        -DE/DX =    0.0             !
! D26   D(3,6,8,11)        -179.995         -DE/DX =    0.0             !
! D27   D(10,6,8,5)         179.3967        -DE/DX =    0.0             !
! D28   D(10,6,8,11)         -0.3128        -DE/DX =    0.0             !
! D29   D(1,12,13,28)         3.1221        -DE/DX =    0.0             !
! D30   D(14,12,13,28)     -177.9762        -DE/DX =    0.0             !
! D31   D(1,12,14,27)         9.7777        -DE/DX =    0.0             !
! D32   D(1,12,14,30)       125.0006        -DE/DX =    0.0             !
! D33   D(13,12,14,27)     -169.1398        -DE/DX =    0.0             !
! D34   D(13,12,14,30)      -53.9169        -DE/DX =    0.0             !
! D35   D(12,14,30,25)      -46.6526        -DE/DX =    0.0             !
! D36   D(27,14,30,25)       69.926         -DE/DX =    0.0             !
! D37   D(20,15,16,17)       -0.5682        -DE/DX =    0.0             !
! D38   D(20,15,16,22)     -179.9582        -DE/DX =    0.0             !
! D39   D(21,15,16,17)      179.8456        -DE/DX =    0.0             !
! D40   D(21,15,16,22)        0.4557        -DE/DX =    0.0             !
! D41   D(16,15,20,19)       -0.3734        -DE/DX =    0.0             !
! D42   D(16,15,20,24)     -178.7775        -DE/DX =    0.0             !
! D43   D(21,15,20,19)      179.2155        -DE/DX =    0.0             !
! D44   D(21,15,20,24)        0.8114        -DE/DX =    0.0             !
! D45   D(15,16,17,18)        0.7435        -DE/DX =    0.0             !
! D46   D(15,16,17,23)     -178.7375        -DE/DX =    0.0             !
! D47   D(22,16,17,18)     -179.8639        -DE/DX =    0.0             !
! D48   D(22,16,17,23)        0.655         -DE/DX =    0.0             !
! D49   D(16,17,18,19)        0.0163        -DE/DX =    0.0             !
! D50   D(16,17,18,25)      179.9581        -DE/DX =    0.0             !
! D51   D(23,17,18,19)      179.5108        -DE/DX =    0.0             !
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! D52   D(23,17,18,25)       -0.5474       -DE/DX =    0.0             !
! D53   D(17,18,19,20)       -0.9602       -DE/DX =    0.0             !
! D54   D(17,18,19,26)       177.1048       -DE/DX =    0.0             !
! D55   D(25,18,19,20)       179.0942       -DE/DX =    0.0             !
! D56   D(25,18,19,26)       -2.8408       -DE/DX =    0.0             !
! D57   D(17,18,25,30)       -69.0981       -DE/DX =    0.0             !
! D58   D(19,18,25,30)       110.8457       -DE/DX =    0.0             !
! D59   D(18,19,20,15)       1.1328       -DE/DX =    0.0             !
! D60   D(18,19,20,24)       179.5756       -DE/DX =    0.0             !
! D61   D(26,19,20,15)       -176.9094       -DE/DX =    0.0             !
! D62   D(26,19,20,24)       1.5333       -DE/DX =    0.0             !
! D63   D(18,19,26,29)       -1.0498       -DE/DX =    0.0             !
! D64   D(20,19,26,29)       177.002       -DE/DX =    0.0             !
! D65   D(18,25,30,14)       -27.1327       -DE/DX =    0.0             !
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GradGradGradG

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.46813	-0.86262	-0.02453
C	-2.37676	-0.68786	-1.0773
C	-1.63748	-0.07942	1.12596
H	-2.28329	-1.28691	-1.98065
C	-3.41835	0.23012	-0.98597
C	-2.66902	0.84787	1.22089
H	-0.92977	-0.16686	1.94715
C	-3.56343	1.00129	0.16459
H	-4.11686	0.34403	-1.80887
H	-2.77324	1.45343	2.1155
H	-4.37033	1.72387	0.23582
B	-0.2786	-1.88247	-0.12167
O	0.25185	-2.52687	0.95554
O	0.34565	-2.18292	-1.31425
C	0.94798	2.62988	-0.21481
C	1.3515	2.12474	-1.44816
C	1.96685	0.87607	-1.51709
C	2.16142	0.13514	-0.35868
C	1.73192	0.63512	0.87779
C	1.1384	1.89115	0.94964
H	0.47235	3.60324	-0.15536
H	1.19593	2.70017	-2.35432
H	2.30602	0.46646	-2.46375
H	0.80706	2.26242	1.91345
O	2.76741	-1.1003	-0.34665
O	1.86766	-0.12548	1.99173
H	0.03922	-1.62479	-2.03374
H	-0.21639	-2.33619	1.77143
H	2.22044	-0.97687	1.68985
H	2.19205	-1.71388	-0.83308

GradGradGradG

Thermal correction to Enthalpy= 0.256472
Thermal correction to Gibbs Free Energy= 0.195071
Sum of electronic and zero-point Energies= -790.496639
Sum of electronic and thermal Energies= -790.480996
Sum of electronic and thermal Enthalpies= -790.480051
Sum of electronic and thermal Free Energies= -790.541452

BDOB-TS1 (TS1-C)

%mem=1GB
%chk=C:\Users\Dell\Desktop\Thusini\Reproducing data of li et. al paper\My comput
er- heteroborole\QST3-BDOB-W1.chk
---
opt=(calcfc,qst3) wb97xd/6-31g(d,p) geom=connectivity

1/5=1,10=4,14=-1,18=20,26=3,27=203,38=1,57=2/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
4//1;
5/5=2,38=5/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1,13=1/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7/10=1,18=20,25=1/1,2,3,16;
1/5=1,10=4,14=-1,18=20,26=3,27=203/3(2);
2/9=110/2;
99//99;
2/9=110/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/5=1,14=-1,18=20,26=3,27=203/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1
C -1.88086 0.75508 -0.14013
C -1.87603 -0.62598 -0.31356

C	-3.04232	-1.35918	-0.3908
C	-4.239	-0.64226	-0.28298
C	-4.24437	0.7419	-0.10759
C	-3.05411	1.47354	-0.03321
H	-3.02572	-2.43399	-0.52856
H	-5.18181	-1.17581	-0.33709
H	-5.19152	1.26405	-0.02544
H	-3.04678	2.54832	0.10437
B	0.19911	0.07663	-0.22411
O	-0.58914	1.21166	-0.10578
O	-0.57872	-1.06674	-0.38862
C	1.74639	0.07687	-0.2557
C	2.4585	-1.11442	-0.45707
C	2.46928	1.26234	-0.06112
C	3.84942	-1.12202	-0.4668
H	1.91587	-2.04305	-0.61044
C	3.86013	1.25933	-0.07049
H	1.93501	2.19432	0.09872
C	4.55053	0.06627	-0.27336
H	4.38622	-2.05188	-0.62533
H	4.40552	2.18539	0.08058
H	5.63617	0.0625	-0.28083
O	0.21709	-0.59681	2.48335
H	1.1671	-0.4967	2.3677
H	0.02529	-1.44996	2.08214

Add virtual bond connecting atoms H27 and O13 Dist= 4.86D+00.

Title Card Required

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-1.6981	0.37737	0.09938
C	-2.55823	-0.69712	0.36399
C	-3.93036	-0.54945	0.18505
C	-4.45798	0.66271	-0.24836
C	-3.60977	1.73358	-0.50822
C	-2.23847	1.58564	-0.32997
H	-4.58687	-1.39075	0.39134
H	-5.52936	0.76357	-0.38212
H	-4.01063	2.68218	-0.84773
H	-1.55307	2.40478	-0.51904
B	0.58619	-0.57985	-0.16403
O	-0.35034	0.32661	0.30752
O	-1.99467	-1.87306	0.78231
C	2.08479	-0.13371	-0.06269

C	3.11153	-1.01452	-0.4297
C	2.44255	1.14222	0.39365
C	4.44817	-0.63755	-0.34509
H	2.85343	-2.00785	-0.78529
C	3.77695	1.52613	0.48369
H	1.66195	1.83976	0.68298
C	4.78185	0.63499	0.11355
H	5.22937	-1.33381	-0.63432
H	4.03476	2.51821	0.84188
H	5.82422	0.93123	0.18414
O	0.28498	-1.78909	-0.69914
H	-0.60921	-2.07909	-0.47098
H	-2.6828	-2.52642	0.94212

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	1.75607	-0.27235	-0.60643
C	1.82636	0.42301	0.60321
C	2.94942	0.41854	1.40791
C	4.05457	-0.31841	0.98101
C	3.99916	-1.01957	-0.2252
C	2.86248	-1.0083	-1.03045
H	2.9687	0.97042	2.34256
H	4.95399	-0.34465	1.58569
H	4.86529	-1.5891	-0.54766
H	2.82439	-1.55146	-1.96771
B	-0.32223	0.80407	-0.57675
O	0.59621	-0.16971	-1.25038
O	0.56397	1.10323	0.8282
C	-1.73408	0.13457	-0.20522
C	-2.83323	0.93536	0.13549
C	-1.90962	-1.25434	-0.16095
C	-4.0553	0.37944	0.50581
H	-2.72775	2.01792	0.10346
C	-3.12715	-1.82233	0.20644
H	-1.07661	-1.89809	-0.43104
C	-4.20404	-1.00495	0.54271
H	-4.89119	1.02338	0.76407
H	-3.23964	-2.90253	0.22872
H	-5.15463	-1.44496	0.82902
O	-0.35536	2.09558	-1.18328
H	-0.99976	2.28773	-1.86843
H	0.26675	2.77215	-0.9061

GradGradGradG

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! R25   R(17,22)         1.0858   1.0853   1.0857 -DE/DX =    0.0         !
! R26   R(19,21)         1.392    1.3933   1.3932 -DE/DX =    0.0         !
! R27   R(19,23)         1.0858   1.0853   1.0858 -DE/DX =    0.0         !
! R28   R(21,24)         1.086    1.0857   1.0859 -DE/DX =    0.0         !
! R29   R(25,26)         0.9639   0.9622   0.9673 -DE/DX =    0.0         !
! R30   R(25,27)         1.2209   0.9621   3.4706 -DE/DX =    0.0         !
! A1    A(2,1,6)        120.6501 121.9512 119.0538 -DE/DX =    0.0         !
! A2    A(2,1,12)       112.7251 109.2939 123.2829 -DE/DX =    0.0         !
! A3    A(6,1,12)       126.622  128.7545 117.5729 -DE/DX =    0.0         !
! A4    A(1,2,3)        122.3229 122.0926 119.9654 -DE/DX =    0.0         !
! A5    A(1,2,13)       110.7773 109.1957 117.6085 -DE/DX =    0.0         !
! A6    A(3,2,13)       126.8993 128.7115 122.4225 -DE/DX =    0.0         !
! A7    A(2,3,4)        117.262  116.51   120.4275 -DE/DX =    0.0         !
! A8    A(2,3,7)        120.7451 121.4116 119.2764 -DE/DX =    0.0         !
! A9    A(4,3,7)        121.9928 122.0783 120.2957 -DE/DX =    0.0         !
! A10   A(3,4,5)        120.7469 121.4204 119.8577 -DE/DX =    0.0         !
! A11   A(3,4,8)        119.4538 119.1783 119.6137 -DE/DX =    0.0         !
! A12   A(5,4,8)        119.7993 119.4013 120.5285 -DE/DX =    0.0         !
! A13   A(4,5,6)        121.4107 121.4783 119.7074 -DE/DX =    0.0         !
! A14   A(4,5,9)        119.4784 119.3712 120.4435 -DE/DX =    0.0         !
! A15   A(6,5,9)        119.1108 119.1505 119.8491 -DE/DX =    0.0         !
! A16   A(1,6,5)        117.6066 116.5472 120.9858 -DE/DX =    0.0         !
! A17   A(1,6,10)       120.5238 121.3671 117.6558 -DE/DX =    0.0         !
! A18   A(5,6,10)       121.8687 122.0854 121.3583 -DE/DX =    0.0         !
! A19   A(12,11,13)     103.2404 111.3789  66.3206 -DE/DX =    0.0         !
! A20   A(12,11,14)     118.4397 124.7384 115.9782 -DE/DX =    0.0         !
! A21   A(12,11,25)     113.2062  96.8001 124.5607 -DE/DX =    0.0         !
! A22   A(13,11,14)     116.5712 123.7893 156.0069 -DE/DX =    0.0         !
! A23   A(14,11,25)     114.049   90.7682 119.4597 -DE/DX =    0.0         !
! A24   A(1,12,11)      109.5542 105.1233 129.7731 -DE/DX =    0.0         !
! A25   A(2,13,11)      103.5439 104.9442  83.6221 -DE/DX =    0.0         !
! A26   A(2,13,27)      110.8523 102.5514 109.8454 -DE/DX =    0.0         !
! A27   A(11,13,27)      71.1116  82.9743 161.4974 -DE/DX =    0.0         !
! A28   A(11,14,15)     122.0706 120.6945 120.3131 -DE/DX =    0.0         !
! A29   A(11,14,16)     119.8174 120.8489 121.6294 -DE/DX =    0.0         !
! A30   A(15,14,16)     118.0992 118.4477 118.0574 -DE/DX =    0.0         !
! A31   A(14,15,17)     121.103  120.8899 121.1661 -DE/DX =    0.0         !
! A32   A(14,15,18)     119.4548 119.5199 119.1005 -DE/DX =    0.0         !
! A33   A(17,15,18)     119.4394 119.5899 119.7334 -DE/DX =    0.0         !
! A34   A(14,16,19)     121.1399 120.851  121.1353 -DE/DX =    0.0         !
! A35   A(14,16,20)     119.2131 119.4955 119.2072 -DE/DX =    0.0         !
! A36   A(19,16,20)     119.6449 119.6535 119.6573 -DE/DX =    0.0         !
! A37   A(15,17,21)     119.9328 119.8407 119.8397 -DE/DX =    0.0         !
! A38   A(15,17,22)     119.9961 120.0182 120.0859 -DE/DX =    0.0         !
! A39   A(21,17,22)     120.0706 120.1412 120.0743 -DE/DX =    0.0         !
! A40   A(16,19,21)     119.8905 119.8905 119.8709 -DE/DX =    0.0         !
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! A41   A(16,19,23)     120.0141  119.9824  120.0753 -DE/DX =    0.0         !
! A42   A(21,19,23)     120.0953  120.1271  120.0538 -DE/DX =    0.0         !
! A43   A(17,21,19)     119.834   120.0801  119.9304 -DE/DX =    0.0         !
! A44   A(17,21,24)     120.067   119.9546  120.0307 -DE/DX =    0.0         !
! A45   A(19,21,24)     120.0983  119.9653  120.0388 -DE/DX =    0.0         !
! A46   A(11,25,26)     110.8461   82.2194  112.3052 -DE/DX =    0.0         !
! A47   A(26,25,27)     114.3471  103.8248   15.0513 -DE/DX =    0.0         !
! A48   A(13,27,25)     128.1738  108.3767   33.4568 -DE/DX =    0.0         !
! D1    D(6,1,2,3)       -0.35     0.0893    0.554  -DE/DX =    0.0         !
! D2    D(6,1,2,13)     179.4095  179.946   179.873  -DE/DX =    0.0         !
! D3    D(12,1,2,3)     179.0705 -179.711   177.0086 -DE/DX =    0.0         !
! D4    D(12,1,2,13)     -1.17     0.1457   -3.6724 -DE/DX =    0.0         !
! D5    D(2,1,6,5)        0.2189    0.0216   -0.5281 -DE/DX =    0.0         !
! D6    D(2,1,6,10)     179.8807  179.8301  179.4301 -DE/DX =    0.0         !
! D7    D(12,1,6,5)    -179.1151  179.7799 -177.1847 -DE/DX =    0.0         !
! D8    D(12,1,6,10)      0.5467   -0.4116    2.7735 -DE/DX =    0.0         !
! D9    D(2,1,12,11)      3.5236   -1.62     54.4512 -DE/DX =    0.0         !
! D10   D(6,1,12,11)   -177.0976  178.5973 -129.0451 -DE/DX =    0.0         !
! D11   D(1,2,3,4)        0.2715   -0.1194   -0.3797 -DE/DX =    0.0         !
! D12   D(1,2,3,7)     -179.8443  179.8388  179.8562 -DE/DX =    0.0         !
! D13   D(13,2,3,4)    -179.4474 -179.9459 -179.6648 -DE/DX =    0.0         !
! D14   D(13,2,3,7)       0.4369    0.0122    0.5711 -DE/DX =    0.0         !
! D15   D(1,2,13,11)     -1.3616    1.387   -13.8485 -DE/DX =    0.0         !
! D16   D(1,2,13,27)     -76.0203   87.3574  179.2151 -DE/DX =    0.0         !
! D17   D(3,2,13,11)     178.3843 -178.7686  165.4525 -DE/DX =    0.0         !
! D18   D(3,2,13,27)     103.7256  -92.7982   -1.4838 -DE/DX =    0.0         !
! D19   D(2,3,4,5)        -0.0809    0.044     0.1678 -DE/DX =    0.0         !
! D20   D(2,3,4,8)      179.8804 -179.9522 -179.9195 -DE/DX =    0.0         !
! D21   D(7,3,4,5)     -179.9636 -179.9138  179.9294 -DE/DX =    0.0         !
! D22   D(7,3,4,8)        -0.0024    0.09     -0.1579 -DE/DX =    0.0         !
! D23   D(3,4,5,6)        -0.0344    0.0645   -0.1352 -DE/DX =    0.0         !
! D24   D(3,4,5,9)     -179.9555 -179.8464  179.9149 -DE/DX =    0.0         !
! D25   D(8,4,5,6)     -179.9955 -179.9393  179.9529 -DE/DX =    0.0         !
! D26   D(8,4,5,9)        0.0834    0.1498    0.0029 -DE/DX =    0.0         !
! D27   D(4,5,6,1)        -0.034    -0.096     0.3208 -DE/DX =    0.0         !
! D28   D(4,5,6,10)    -179.6909 -179.903  -179.6358 -DE/DX =    0.0         !
! D29   D(9,5,6,1)      179.8874  179.8151 -179.729  -DE/DX =    0.0         !
! D30   D(9,5,6,10)       0.2304    0.0082    0.3144 -DE/DX =    0.0         !
! D31   D(13,11,12,1)    -4.0042    2.5629  -42.5251 -DE/DX =    0.0         !
! D32   D(14,11,12,1)  -134.5477  179.1538  163.8346 -DE/DX =    0.0         !
! D33   D(25,11,12,1)    88.0232  -85.1578  -15.722  -DE/DX =    0.0         !
! D34   D(12,11,13,2)     3.2328   -2.4741   30.9784 -DE/DX =    0.0         !
! D35   D(12,11,13,27)  110.9645 -103.6447  168.9145 -DE/DX =    0.0         !
! D36   D(14,11,13,2)   134.8916 -179.1033  131.9873 -DE/DX =    0.0         !
! D37   D(14,11,13,27) -117.3767   79.7261  -90.0766 -DE/DX =    0.0         !
! D38   D(12,11,14,15) -156.2982 -176.2346  175.7315 -DE/DX =    0.0         !
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 ! D39   D(12,11,14,16)    25.0282    4.8686   -4.1791 -DE/DX =    0.0         !
 ! D40   D(13,11,14,15)    79.5005   -0.055    85.9569 -DE/DX =    0.0         !
 ! D41   D(13,11,14,16)   -99.1731 -178.9517  -93.9537 -DE/DX =    0.0         !
 ! D42   D(25,11,14,15)   -19.2098   84.9415   -4.6878 -DE/DX =    0.0         !
 ! D43   D(25,11,14,16)   162.1165  -93.9553  175.4016 -DE/DX =    0.0         !
 ! D44   D(12,11,25,26)     9.5449 -120.6979  -18.1276 -DE/DX =    0.0         !
 ! D45   D(14,11,25,26)  -129.8075    4.438   162.3302 -DE/DX =    0.0         !
 ! D46   D(2,13,27,25)    101.134   -78.3102  126.471  -DE/DX =    0.0         !
 ! D47   D(11,13,27,25)     3.402    25.5028   -8.4687 -DE/DX =    0.0         !
 ! D48   D(11,14,15,17)  -178.4375 -179.0566 -179.9134 -DE/DX =    0.0         !
 ! D49   D(11,14,15,18)     2.184     1.1279    0.0576 -DE/DX =    0.0         !
 ! D50   D(16,14,15,17)     0.2579   -0.1339    0.0003 -DE/DX =    0.0         !
 ! D51   D(16,14,15,18)  -179.1206 -179.9493  179.9713 -DE/DX =    0.0         !
 ! D52   D(11,14,16,19)   178.5377  179.0738  179.7867 -DE/DX =    0.0         !
 ! D53   D(11,14,16,20)    -1.9952   -0.9356   -0.0867 -DE/DX =    0.0         !
 ! D54   D(15,14,16,19)    -0.1882    0.1527   -0.1258 -DE/DX =    0.0         !
 ! D55   D(15,14,16,20)   179.279  -179.8566 -179.9992 -DE/DX =    0.0         !
 ! D56   D(14,15,17,21)    -0.1193    0.0553    0.1135 -DE/DX =    0.0         !
 ! D57   D(14,15,17,22)  -179.86   -179.9118 -179.9794 -DE/DX =    0.0         !
 ! D58   D(18,15,17,21)   179.2594  179.8707 -179.8573 -DE/DX =    0.0         !
 ! D59   D(18,15,17,22)    -0.4814   -0.0965    0.0498 -DE/DX =    0.0         !
 ! D60   D(14,16,19,21)    -0.0201   -0.0931    0.1368 -DE/DX =    0.0         !
 ! D61   D(14,16,19,23)   179.8696  179.9363 -179.8525 -DE/DX =    0.0         !
 ! D62   D(20,16,19,21)  -179.485   179.9163 -179.9904 -DE/DX =    0.0         !
 ! D63   D(20,16,19,23)     0.4047   -0.0544    0.0203 -DE/DX =    0.0         !
 ! D64   D(15,17,21,19)    -0.0957    0.0076   -0.1033 -DE/DX =    0.0         !
 ! D65   D(15,17,21,24)  -179.7947 -179.986   179.7842 -DE/DX =    0.0         !
 ! D66   D(22,17,21,19)   179.6449  179.9747  179.9897 -DE/DX =    0.0         !
 ! D67   D(22,17,21,24)    -0.0541   -0.0189   -0.1228 -DE/DX =    0.0         !
 ! D68   D(16,19,21,17)     0.1643    0.0111   -0.0201 -DE/DX =    0.0         !
 ! D69   D(16,19,21,24)   179.8633 -179.9953 -179.9076 -DE/DX =    0.0         !
 ! D70   D(23,19,21,17)  -179.7253  179.9817  179.9692 -DE/DX =    0.0         !
 ! D71   D(23,19,21,24)    -0.0263   -0.0247    0.0817 -DE/DX =    0.0         !
 ! D72   D(26,25,27,13)  -109.5514  -91.5892 -133.2494 -DE/DX =    0.0         !
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```

GradGradGradG

phase.chk
---
freq wb97xd/6-31g(d,p) geom=connectivity

1/10=4,30=1,38=1,57=2/1,3;
2/12=2,17=6,18=5,40=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
4//1;
5/5=2,38=5,98=1/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1/2;
6/7=2,8=2,9=2,10=2,18=1,28=1/1;
7/8=1,10=1,25=1/1,2,3,16;
1/10=4,30=1/3;
99//99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	1.78023	-0.4216	-0.53906
C	1.82247	0.45075	0.54795
C	2.9548	0.61736	1.31544
C	4.08555	-0.12661	0.95969
C	4.05225	-0.9967	-0.12658
C	2.89547	-1.15826	-0.89587
H	2.95841	1.30097	2.15677
H	4.99674	-0.02151	1.53829
H	4.94069	-1.56403	-0.3837
H	2.85979	-1.83716	-1.73998
B	-0.30367	0.50825	-0.51861
O	0.56427	-0.44823	-1.14349
O	0.60411	1.08974	0.71302
C	-1.77028	0.06861	-0.1643
C	-2.80971	0.99511	-0.02052
C	-2.05998	-1.28493	0.04436
C	-4.09383	0.5866	0.32509
H	-2.61276	2.04968	-0.19141
C	-3.3421	-1.70157	0.38886
H	-1.26949	-2.02075	-0.07404
C	-4.36127	-0.76419	0.53138
H	-4.88727	1.32048	0.42959
H	-3.54695	-2.75645	0.54435
H	-5.36366	-1.08585	0.79798
O	-0.20097	1.9337	-1.14576

H 0.32319 1.91567 -1.95453
H 0.45878 1.9684 -0.11907

GradGradGradG

7/10=1,18=20,25=1/1,2,3,16;
1/10=4,14=-1,18=10,26=3,44=3/23(2);
2/29=1/2;
99/5=20/99;
2/29=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1,13=1/2;
7/10=1,18=20,25=1/1,2,3,16;
1/14=-1,18=10,26=3,44=3/23(-8);
2/29=1/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/5=20,9=1/99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	1.78023	-0.4216	-0.53906
C	1.82247	0.45075	0.54795
C	2.9548	0.61736	1.31544
C	4.08555	-0.12661	0.95969
C	4.05225	-0.9967	-0.12658
C	2.89547	-1.15826	-0.89587
H	2.95841	1.30097	2.15677
H	4.99674	-0.02151	1.53829
H	4.94069	-1.56403	-0.3837
H	2.85979	-1.83716	-1.73998
B	-0.30367	0.50825	-0.51861
O	0.56427	-0.44823	-1.14349
O	0.60411	1.08974	0.71302
C	-1.77028	0.06861	-0.1643
C	-2.80971	0.99511	-0.02052
C	-2.05998	-1.28493	0.04436
C	-4.09383	0.5866	0.32509
H	-2.61276	2.04968	-0.19141
C	-3.3421	-1.70157	0.38886
H	-1.26949	-2.02075	-0.07404
C	-4.36127	-0.76419	0.53138
H	-4.88727	1.32048	0.42959
H	-3.54695	-2.75645	0.54435
H	-5.36366	-1.08585	0.79798
O	-0.20097	1.9337	-1.14576

H 0.32319 1.91567 -1.95453
H 0.45878 1.9684 -0.11907

IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC

INPUT DATA FOR L123

GENERAL PARAMETERS:
Follow reaction path in both directions.
Maximum points per path = 10
Step size = 0.100 bohr
Integration scheme = HPC
Redo corrector integration= Yes
DWI Weight Power = 2
DWI will use Hessian update vectors when possible.
Max correction cycles = 20
Initial Hessian = CalcFC
Hessian evaluation = All updating
Hessian updating method = Bofill

IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC

Benzodioxaborole TS2 **TS2-C**

****

%mem=1GB
%nprocshared=4
Will use up to 4 processors via shared memory.
%chk=T:\CHM\deg013\Thusini\Reproducing data of li et. al paper\BDOB-Gas phase-7-
16\Gas phase product formation-Gas phase\OPT-QST3-Trial3-8-17-BDOB product form-
using-INT_W1-Correct cat donating H product and 27 kcalTS2.chk

---

opt=(calcall,qst3) wb97xd/6-31g(d,p) geom=connectivity

1/5=1,10=4,14=-1,18=20,26=3,27=203,38=1,57=2/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
4//1;
5/5=2,38=5/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1/2;

6/7=2,8=2,9=2,10=2,18=1,28=1/1;
7/10=1,25=1/1,2,3,16;
1/5=1,10=4,14=-1,18=20,26=3,27=203/3(3);
2/9=110/2;
7/8=1,9=1,25=1,44=-1/16;
99//99;
2/9=110/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1/2;
7/10=1,25=1/1,2,3,16;
1/5=1,10=4,14=-1,18=20,26=3,27=203/3(-8);
2/9=110/2;
6/7=2,8=2,9=2,10=2,18=1,19=2,28=1/1;
7/8=1,9=1,25=1,44=-1/16;
99//99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	1.74794	0.22261	-0.43455
C	2.5128	-0.92015	-0.15907
C	3.88955	-0.80673	-0.0046
C	4.51063	0.4352	-0.12002
C	3.75744	1.56719	-0.40106
C	2.37705	1.45652	-0.56113
H	4.47847	-1.69491	0.21064
H	5.58503	0.5092	0.00768
H	4.23557	2.53506	-0.50192
H	1.77056	2.32489	-0.79788
C	-2.02992	0.38965	-0.04401
C	-3.02568	0.86921	0.8177
C	-2.42419	-0.35716	-1.16266
C	-4.37038	0.61684	0.56907
H	-2.73368	1.4425	1.69249
C	-3.76807	-0.61158	-1.41782
H	-1.66419	-0.73818	-1.83894
C	-4.74226	-0.12375	-0.55059
H	-5.12914	0.99339	1.24816
H	-4.05695	-1.18867	-2.29099
H	-5.792	-0.32134	-0.74604
O	0.40306	0.0767	-0.59972

B	-0.52004	0.65848	0.26117
O	-0.17288	1.49071	1.27603
H	0.77356	1.51901	1.44422
O	1.84823	-2.10697	-0.06797
H	2.45651	-2.79379	0.2192
O	-0.42746	-1.78438	1.71286
H	-1.30111	-1.72482	1.31573
H	0.16051	-1.99027	0.97463

Add virtual bond connecting atoms H30 and O26 Dist= 3.76D+00.

Title Card Required

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	2.10744	0.12143	-0.37274
C	1.67795	0.6214	0.86372
C	1.08443	1.87743	0.93557
C	0.89401	2.61617	-0.22887
C	1.29753	2.11103	-1.46222
C	1.91288	0.86236	-1.53116
H	0.75308	2.24871	1.89939
H	0.41837	3.58953	-0.16942
H	1.14196	2.68645	-2.36839
H	2.25204	0.45275	-2.47781
C	-1.41416	-0.84891	-0.01046
C	-2.32279	-0.67415	-1.06324
C	-1.58351	-0.06571	1.14002
C	-3.36438	0.24383	-0.9719
H	-2.22932	-1.2732	-1.96659
C	-2.61505	0.86158	1.23495
H	-0.8758	-0.15315	1.96122
C	-3.50946	1.015	0.17865
H	-4.06289	0.35774	-1.79481
H	-2.71926	1.46714	2.12957
H	-4.31636	1.73758	0.24988
O	2.71343	-1.11401	-0.36071
B	-0.22463	-1.86876	-0.1076
O	0.39962	-2.16921	-1.30019
H	0.09319	-1.61108	-2.01968
O	1.81369	-0.13919	1.97766
H	2.16647	-0.99058	1.67578
O	0.30582	-2.51316	0.9696
H	-0.16242	-2.32248	1.78549
H	2.13808	-1.72759	-0.84714

Add virtual bond connecting atoms H30 and O24 Dist= 3.50D+00.

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	1.69374	-0.24594	-0.56922
C	2.79278	0.5498	-0.22506
C	4.00911	-0.0466	0.08271
C	4.13104	-1.43494	0.0605
C	3.03885	-2.22562	-0.27425
C	1.82122	-1.62631	-0.59075
H	4.86151	0.57443	0.34817
H	5.08467	-1.89118	0.30353
H	3.13134	-3.30601	-0.29559
H	0.95215	-2.21428	-0.86687
C	-2.08883	0.22739	0.2343
C	-2.27319	-1.12797	0.54008
C	-3.19098	0.94394	-0.24226
C	-3.50862	-1.74638	0.37869
H	-1.43108	-1.71515	0.90382
C	-4.43226	0.33415	-0.40553
H	-3.06964	1.99489	-0.48866
C	-4.59366	-1.01286	-0.09523
H	-3.62739	-2.79926	0.617
H	-5.27513	0.90976	-0.77661
H	-5.56005	-1.49084	-0.224
O	0.50019	0.33538	-0.8908
B	-0.67026	0.89764	0.45487
O	-0.04634	0.83901	1.70286
H	-0.53215	0.28162	2.31129
O	2.5908	1.90054	-0.22319
H	3.41113	2.34282	0.01002
O	-0.51545	2.31091	-0.15781
H	0.01043	2.83275	0.46087
H	0.37408	1.56228	-0.9381

GradGradGradG

Maximum Displacement 0.000760 0.001800 YES
RMS Displacement 0.000169 0.001200 YES
Predicted change in Energy=-1.281463D-09
Optimization completed.
-- Stationary point found.

! Optimized Parameters !
! (Angstroms and Degrees) !

Name	Definition	TS	Reactant	Product	Derivative Info.
R1	R(1,2)	1.3998	1.4024	1.4012	-DE/DX = 0.0
R2	R(1,6)	1.3864	1.3908	1.3888	-DE/DX = 0.0
R3	R(1,22)	1.366	1.3628	1.3761	-DE/DX = 0.0
R4	R(2,3)	1.3892	1.39	1.3911	-DE/DX = 0.0
R5	R(2,26)	1.3658	1.3633	1.3557	-DE/DX = 0.0
R6	R(3,4)	1.3939	1.3934	1.3921	-DE/DX = 0.0
R7	R(3,7)	1.0875	1.0872	1.0847	-DE/DX = 0.0
R8	R(4,5)	1.3893	1.3884	1.3925	-DE/DX = 0.0
R9	R(4,8)	1.0847	1.0845	1.085	-DE/DX = 0.0
R10	R(5,6)	1.3935	1.394	1.3938	-DE/DX = 0.0
R11	R(5,9)	1.0845	1.0842	1.0846	-DE/DX = 0.0
R12	R(6,10)	1.085	1.0853	1.0858	-DE/DX = 0.0
R13	R(11,12)	1.4016	1.4014	1.4016	-DE/DX = 0.0
R14	R(11,13)	1.3983	1.4016	1.402	-DE/DX = 0.0
R15	R(11,23)	1.5844	1.5637	1.5699	-DE/DX = 0.0
R16	R(12,14)	1.391	1.3906	1.3914	-DE/DX = 0.0
R17	R(12,15)	1.0891	1.0859	1.088	-DE/DX = 0.0
R18	R(13,16)	1.3926	1.3913	1.3903	-DE/DX = 0.0
R19	R(13,17)	1.0862	1.0863	1.0876	-DE/DX = 0.0
R20	R(14,18)	1.3928	1.393	1.3927	-DE/DX = 0.0
R21	R(14,19)	1.086	1.0857	1.0854	-DE/DX = 0.0
R22	R(16,18)	1.3917	1.3925	1.3926	-DE/DX = 0.0
R23	R(16,20)	1.086	1.0858	1.0853	-DE/DX = 0.0
R24	R(18,21)	1.0858	1.0859	1.0855	-DE/DX = 0.0
R25	R(22,23)	1.6608	1.3899	3.044	-DE/DX = 0.0
R26	R(22,30)	1.2343	2.6096	0.9717	-DE/DX = 0.0
R27	R(23,24)	1.3965	1.3576	1.3792	-DE/DX = 0.0
R28	R(23,28)	1.5482	2.8432	1.3627	-DE/DX = 0.0
R29	R(24,25)	0.9575	0.9617	0.9608	-DE/DX = 0.0
R30	R(24,30)	2.6278	3.5099	1.85	-DE/DX = 0.0
R31	R(26,27)	0.9607	0.9613	0.9698	-DE/DX = 0.0
R32	R(26,30)	2.3538	1.9872	3.257	-DE/DX = 0.0
R33	R(28,29)	0.9652	0.9615	0.9598	-DE/DX = 0.0
R34	R(28,30)	1.2011	0.966	2.6972	-DE/DX = 0.0
A1	A(2,1,6)	119.8413	119.6107	120.1818	-DE/DX = 0.0

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! A2    A(2,1,22)      120.1344  118.3449  116.5911 -DE/DX =    0.0        !
! A3    A(6,1,22)      120.0232  122.0278  123.227  -DE/DX =    0.0        !
! A4    A(1,2,3)       119.8578  119.7042  119.9045 -DE/DX =    0.0        !
! A5    A(1,2,26)      116.5164  117.1707  119.6181 -DE/DX =    0.0        !
! A6    A(3,2,26)      123.6245  123.1225  120.4559 -DE/DX =    0.0        !
! A7    A(2,3,4)       120.0446  120.3318  119.6244 -DE/DX =    0.0        !
! A8    A(2,3,7)       119.6818  119.4627  119.0312 -DE/DX =    0.0        !
! A9    A(4,3,7)       120.2718  120.2051  121.3209 -DE/DX =    0.0        !
! A10   A(3,4,5)       120.1282  120.1102  120.5784 -DE/DX =    0.0        !
! A11   A(3,4,8)       119.4905  119.5155  119.3536 -DE/DX =    0.0        !
! A12   A(5,4,8)       120.3811  120.3739  120.0657 -DE/DX =    0.0        !
! A13   A(4,5,6)       119.7935  119.7155  119.7837 -DE/DX =    0.0        !
! A14   A(4,5,9)       120.307   120.4919  120.3935 -DE/DX =    0.0        !
! A15   A(6,5,9)       119.8986  119.7919  119.8214 -DE/DX =    0.0        !
! A16   A(1,6,5)       120.3319  120.5228  119.9053 -DE/DX =    0.0        !
! A17   A(1,6,10)      118.0245  118.485   118.8289 -DE/DX =    0.0        !
! A18   A(5,6,10)      121.6418  120.9884  121.265  -DE/DX =    0.0        !
! A19   A(12,11,13)    117.7886  118.2418  117.9309 -DE/DX =    0.0        !
! A20   A(12,11,23)    119.7652  120.4802  121.7178 -DE/DX =    0.0        !
! A21   A(13,11,23)    122.4396  121.2636  120.3445 -DE/DX =    0.0        !
! A22   A(11,12,14)    121.4289  121.0002  121.2155 -DE/DX =    0.0        !
! A23   A(11,12,15)    119.5039  119.0074  119.9553 -DE/DX =    0.0        !
! A24   A(14,12,15)    119.0649  119.992   118.8227 -DE/DX =    0.0        !
! A25   A(11,13,16)    121.207   121.0302  121.2132 -DE/DX =    0.0        !
! A26   A(11,13,17)    119.0157  119.139   119.741  -DE/DX =    0.0        !
! A27   A(16,13,17)    119.7773  119.8306  119.0036 -DE/DX =    0.0        !
! A28   A(12,14,18)    119.8185  119.8913  119.838  -DE/DX =    0.0        !
! A29   A(12,14,19)    120.1791  120.0696  120.0821 -DE/DX =    0.0        !
! A30   A(18,14,19)    120.0019  120.0388  120.0799 -DE/DX =    0.0        !
! A31   A(13,16,18)    120.0701  119.8317  119.8823 -DE/DX =    0.0        !
! A32   A(13,16,20)    119.9844  120.1092  119.9777 -DE/DX =    0.0        !
! A33   A(18,16,20)    119.9455  120.0591  120.1394 -DE/DX =    0.0        !
! A34   A(14,18,16)    119.6867  120.0042  119.9169 -DE/DX =    0.0        !
! A35   A(14,18,21)    120.1243  119.9657  120.0168 -DE/DX =    0.0        !
! A36   A(16,18,21)    120.1888  120.0302  120.0658 -DE/DX =    0.0        !
! A37   A(1,22,23)     120.3621  122.3803   78.363  -DE/DX =    0.0        !
! A38   A(1,22,30)     121.4213   95.9351  107.5653 -DE/DX =    0.0        !
! A39   A(11,23,22)    109.4515  116.645   125.129  -DE/DX =    0.0        !
! A40   A(11,23,24)    120.4402  119.8806  122.5463 -DE/DX =    0.0        !
! A41   A(11,23,28)    114.8714   89.0474  123.589  -DE/DX =    0.0        !
! A42   A(22,23,24)    110.5371  123.3532   62.951  -DE/DX =    0.0        !
! A43   A(24,23,28)    110.3277   97.8565  113.849  -DE/DX =    0.0        !
! A44   A(23,24,25)    111.4437  113.6056  112.1251 -DE/DX =    0.0        !
! A45   A(23,24,30)     35.8597   49.6184   99.2985 -DE/DX =    0.0        !
! A46   A(25,24,30)    146.3299   87.1754  110.1474 -DE/DX =    0.0        !
! A47   A(2,26,27)     109.2301  109.4801  105.8551 -DE/DX =    0.0        !
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! A48   A(2,26,30)       89.8088  113.4498   64.5911 -DE/DX =    0.0         !
! A49   A(27,26,30)      160.7601  115.0      42.745  -DE/DX =    0.0         !
! A50   A(23,28,29)      107.1152   72.9209  112.8367 -DE/DX =    0.0         !
! A51   A(29,28,30)      107.483   104.5135  147.7892 -DE/DX =    0.0         !
! A52   A(22,30,24)       71.1748   43.5378  146.0745 -DE/DX =    0.0         !
! A53   A(26,30,28)      110.6693  158.5021   59.3486 -DE/DX =    0.0         !
! D1    D(6,1,2,3)        0.5246    0.5218   -1.5667 -DE/DX =    0.0         !
! D2    D(6,1,2,26)    -179.8809 -178.9041  176.7527 -DE/DX =    0.0         !
! D3    D(22,1,2,3)    -179.0974  179.0724  178.5186 -DE/DX =    0.0         !
! D4    D(22,1,2,26)      0.4971   -0.3535   -3.162  -DE/DX =    0.0         !
! D5    D(2,1,6,5)       -0.1377   -0.7457    0.4718 -DE/DX =    0.0         !
! D6    D(2,1,6,10)    -179.6735  178.5594 -179.8445 -DE/DX =    0.0         !
! D7    D(22,1,6,5)     179.4847 -179.241  -179.6194 -DE/DX =    0.0         !
! D8    D(22,1,6,10)     -0.051     0.0641    0.0643 -DE/DX =    0.0         !
! D9    D(2,1,22,23)    -81.4904  116.1335   77.4395 -DE/DX =    0.0         !
! D10   D(2,1,22,30)      2.9213   29.4434  114.2763 -DE/DX =    0.0         !
! D11   D(6,1,22,23)     98.8883  -65.3529 -102.4723 -DE/DX =    0.0         !
! D12   D(6,1,22,30)   -176.7    -152.043   -65.6355 -DE/DX =    0.0         !
! D13   D(1,2,3,4)       -0.5799    0.1027    1.4621 -DE/DX =    0.0         !
! D14   D(1,2,3,7)      179.9048  179.891   179.7231 -DE/DX =    0.0         !
! D15   D(26,2,3,4)     179.8559  179.4929 -176.843  -DE/DX =    0.0         !
! D16   D(26,2,3,7)       0.3405   -0.7189    1.4181 -DE/DX =    0.0         !
! D17   D(1,2,26,27)    -178.9567 -173.6828   -3.7261 -DE/DX =    0.0         !
! D18   D(1,2,26,30)      -1.7855  -43.7362  -15.1775 -DE/DX =    0.0         !
! D19   D(3,2,26,27)      0.621     6.9127  174.5838 -DE/DX =    0.0         !
! D20   D(3,2,26,30)    177.7922  136.8592  163.1324 -DE/DX =    0.0         !
! D21   D(2,3,4,5)        0.2489   -0.5112   -0.2774 -DE/DX =    0.0         !
! D22   D(2,3,4,8)     -179.9249  179.7087  179.1713 -DE/DX =    0.0         !
! D23   D(7,3,4,5)      179.7614  179.7021 -178.4976 -DE/DX =    0.0         !
! D24   D(7,3,4,8)       -0.4124   -0.0779    0.9511 -DE/DX =    0.0         !
! D25   D(3,4,5,6)        0.1388    0.29     -0.8156 -DE/DX =    0.0         !
! D26   D(3,4,5,9)      179.7995 -179.3913  179.6074 -DE/DX =    0.0         !
! D27   D(8,4,5,6)     -179.6857 -179.9318  179.7396 -DE/DX =    0.0         !
! D28   D(8,4,5,9)       -0.0251    0.3868    0.1626 -DE/DX =    0.0         !
! D29   D(4,5,6,1)       -0.1936    0.3406    0.7137 -DE/DX =    0.0         !
! D30   D(4,5,6,10)     179.325  -178.9469 -178.9621 -DE/DX =    0.0         !
! D31   D(9,5,6,1)     -179.8557 -179.9759 -179.7068 -DE/DX =    0.0         !
! D32   D(9,5,6,10)      -0.3371    0.7367    0.6174 -DE/DX =    0.0         !
! D33   D(13,11,12,14)   -0.0609   -0.25     -0.201  -DE/DX =    0.0         !
! D34   D(13,11,12,15)   179.3896  179.5176 -179.2632 -DE/DX =    0.0         !
! D35   D(23,11,12,14)   179.0258 -178.8861 -179.255  -DE/DX =    0.0         !
! D36   D(23,11,12,15)    -1.5237    0.8815    1.6828 -DE/DX =    0.0         !
! D37   D(12,11,13,16)     0.1465    0.334    -0.3329 -DE/DX =    0.0         !
! D38   D(12,11,13,17)  -179.794   -179.8442 -177.9469 -DE/DX =    0.0         !
! D39   D(23,11,13,16)  -178.9142  178.9588  178.7347 -DE/DX =    0.0         !
! D40   D(23,11,13,17)     1.1453   -1.2194    1.1207 -DE/DX =    0.0         !
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 ! D41   D(12,11,23,22)    74.6189  176.1226  109.2902 -DE/DX =    0.0         !
 ! D42   D(12,11,23,24)   -55.1034   -7.7441   31.4474 -DE/DX =    0.0         !
 ! D43   D(12,11,23,28)   169.1274   90.7737 -150.0858 -DE/DX =    0.0         !
 ! D44   D(13,11,23,22)  -106.3385   -2.4717  -69.7414 -DE/DX =    0.0         !
 ! D45   D(13,11,23,24)   123.9392  173.6616 -147.5842 -DE/DX =    0.0         !
 ! D46   D(13,11,23,28)   -11.8299  -87.8206   30.8826 -DE/DX =    0.0         !
 ! D47   D(11,12,14,18)    -0.0541    0.0439    0.479  -DE/DX =    0.0         !
 ! D48   D(11,12,14,19)   179.6794  179.8356 -179.4424 -DE/DX =    0.0         !
 ! D49   D(15,12,14,18)  -179.5069 -179.7214  179.5516 -DE/DX =    0.0         !
 ! D50   D(15,12,14,19)     0.2266    0.0703   -0.3698 -DE/DX =    0.0         !
 ! D51   D(11,13,16,18)    -0.1172   -0.2111    0.5856 -DE/DX =    0.0         !
 ! D52   D(11,13,16,20)   179.9625  179.7656 -179.1511 -DE/DX =    0.0         !
 ! D53   D(17,13,16,18)   179.8228  179.9683  178.2169 -DE/DX =    0.0         !
 ! D54   D(17,13,16,20)    -0.0974   -0.0549   -1.5199 -DE/DX =    0.0         !
 ! D55   D(12,14,18,16)     0.0859    0.086    -0.2239 -DE/DX =    0.0         !
 ! D56   D(12,14,18,21)   179.9426 -179.9855  179.5198 -DE/DX =    0.0         !
 ! D57   D(19,14,18,16)  -179.6481 -179.7058  179.6975 -DE/DX =    0.0         !
 ! D58   D(19,14,18,21)     0.2086    0.2227   -0.5588 -DE/DX =    0.0         !
 ! D59   D(13,16,18,14)    -0.0018   -0.0034   -0.3007 -DE/DX =    0.0         !
 ! D60   D(13,16,18,21)  -179.8584 -179.9318  179.9557 -DE/DX =    0.0         !
 ! D61   D(20,16,18,14)   179.9185 -179.9802  179.4356 -DE/DX =    0.0         !
 ! D62   D(20,16,18,21)     0.0619    0.0914   -0.3079 -DE/DX =    0.0         !
 ! D63   D(1,22,23,11)   -125.0256 -179.2874   -2.4844 -DE/DX =    0.0         !
 ! D64   D(1,22,23,24)      9.891     4.7267  109.808  -DE/DX =    0.0         !
 ! D65   D(1,22,30,24)    -83.8896   94.3619  -31.8324 -DE/DX =    0.0         !
 ! D66   D(11,23,24,25)     6.4762  173.8729    6.8315 -DE/DX =    0.0         !
 ! D67   D(11,23,24,30)   175.8793  110.1223  123.1483 -DE/DX =    0.0         !
 ! D68   D(22,23,24,25)  -122.7666  -10.2651 -109.3098 -DE/DX =    0.0         !
 ! D69   D(28,23,24,25)   144.0308   80.4372 -171.772  -DE/DX =    0.0         !
 ! D70   D(28,23,24,30)   -46.5661   16.6865  -55.4552 -DE/DX =    0.0         !
 ! D71   D(11,23,28,29)   141.8968    4.9645    3.8389 -DE/DX =    0.0         !
 ! D72   D(24,23,28,29)     1.7887  125.0102 -177.5742 -DE/DX =    0.0         !
 ! D73   D(23,24,30,22)   -75.4277   38.3804  -37.5789 -DE/DX =    0.0         !
 ! D74   D(25,24,30,22)   -57.4444  -86.2505   80.2343 -DE/DX =    0.0         !
 ! D75   D(2,26,30,28)    134.8829  -51.7759 -123.6078 -DE/DX =    0.0         !
 ! D76   D(27,26,30,28)   -53.2464   75.3343   72.7348 -DE/DX =    0.0         !
 ! D77   D(29,28,30,26)     1.3713  156.5383   10.1644 -DE/DX =    0.0         !
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GradGradGradG

%chk=T:\CHM\deg013\Thusini\Reproducing data of li et. al paper\BDOB-Gas phase-7-
16\Gas phase product formation-Gas phase\FREQ-QST3-TRIAL3-8-17-BDOB PRODUCT FORM
-USING-INT_W1-CORRECT CAT DONATING H PRODUCT AND 27 KCALTS2.chk
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freq wb97xd/6-31g(d,p) geom=connectivity

1/10=4,30=1,38=1,57=2/1,3;
2/12=2,17=6,18=5,40=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
4//1;
5/5=2,38=5,98=1/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1/2;
6/7=2,8=2,9=2,10=2,18=1,28=1/1;
7/8=1,10=1,25=1/1,2,3,16;
1/10=4,30=1/3;
99//99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.62832	0.21459	-0.49397
C	-2.72722	-0.58132	-0.14976
C	-3.94362	0.01489	0.15808
C	-4.06578	1.40322	0.13586
C	-2.97373	2.19407	-0.19895
C	-1.75602	1.59494	-0.5155
H	-4.79591	-0.60627	0.4236
H	-5.01946	1.85931	0.37894
H	-3.0664	3.27444	-0.2203
H	-0.88706	2.18305	-0.79164
C	2.0234	-0.19592	0.15898
C	2.20771	1.1595	0.46448
C	3.12565	-0.91259	-0.31719
C	3.44317	1.77787	0.30322
H	1.36551	1.74677	0.82789
C	4.36698	-0.30285	-0.48033
H	3.00435	-1.96359	-0.56338
C	4.52832	1.04423	-0.17029
H	3.56191	2.8308	0.54132
H	5.20992	-0.87854	-0.85109

H	5.49475	1.52216	-0.29893
O	-0.43465	-0.36647	-0.81558
B	0.60477	-0.86608	0.37947
O	-0.01914	-0.80744	1.62748
H	0.46692	-0.25038	2.23602
O	-2.52507	-1.93204	-0.14789
H	-3.34535	-2.37443	0.08527
O	0.44993	-2.27935	-0.23335
H	-0.07646	-2.801	0.38506
H	-0.30838	-1.59333	-0.86333

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.
Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-07
Number of steps in this run= 2 maximum allowed number of steps= 2.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

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- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.234547 (Hartree/Particle)
Thermal correction to Energy= 0.249637
Thermal correction to Enthalpy= 0.250581
Thermal correction to Gibbs Free Energy= 0.191076
Sum of electronic and zero-point Energies= -790.453767
Sum of electronic and thermal Energies= -790.438677
Sum of electronic and thermal Enthalpies= -790.437732
Sum of electronic and thermal Free Energies= -790.497237

BENZODIAZABOROLE 3.1D

%mem=1GB
%chk=T:\CHM\deg013\Thusini\Reproducing data of li et. al paper\-BDAB-1st reactio
n7-20\TPH-01-46-OPT-BDAB-Gas phase.chk
---
opt wb97xd/6-31g(d,p) geom=connectivity

1/14=-1,18=20,19=15,26=3,38=1,57=2/1,3;

2/9=110,12=2,17=6,18=5,40=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4//1;
5/5=2,38=5/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(2);
2/9=110/2;
99//99;
2/9=110/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.91223	0.6964	0.11066
C	-1.91223	-0.69639	-0.11067
C	-3.10473	-1.39845	-0.22656
C	-4.30092	-0.68897	-0.11242
C	-4.30092	0.68897	0.11244
C	-3.10474	1.39845	0.22656
H	-3.10422	-2.47021	-0.39945
H	-5.24434	-1.21792	-0.20001
H	-5.24434	1.21791	0.20004
H	-3.10422	2.47021	0.39946
B	0.28106	0.	-0.00001
C	1.84079	0.	0.
C	2.56692	1.16502	-0.28689
C	2.56691	-1.16501	0.28689
C	3.95831	1.16959	-0.28875
H	2.03687	2.0842	-0.52423
C	3.9583	-1.16959	0.28876
H	2.03686	-2.08419	0.52422
C	4.65728	0.	0.00001
H	4.49756	2.08383	-0.51681
H	4.49755	-2.08384	0.51683
H	5.74296	-0.00001	0.00001
N	-0.59084	1.12465	0.17438

H	-0.36237	2.0847	0.36929
N	-0.59084	-1.12464	-0.17441
H	-0.36237	-2.08469	-0.36931

GradGradGradG

```
! R22   R(15,19)          1.3922       -DE/DX =    0.0            !
! R23   R(15,20)          1.0857       -DE/DX =    0.0            !
! R24   R(17,19)          1.3922       -DE/DX =    0.0            !
! R25   R(17,21)          1.0857       -DE/DX =    0.0            !
! R26   R(19,22)          1.0857       -DE/DX =    0.0            !
! R27   R(23,24)          1.0052       -DE/DX =    0.0            !
! R28   R(25,26)          1.0052       -DE/DX =    0.0            !
! A1    A(2,1,6)         120.8142      -DE/DX =    0.0            !
! A2    A(2,1,23)         108.1164      -DE/DX =    0.0            !
! A3    A(6,1,23)         131.0693      -DE/DX =    0.0            !
! A4    A(1,2,3)         120.8142      -DE/DX =    0.0            !
! A5    A(1,2,25)         108.1164      -DE/DX =    0.0            !
! A6    A(3,2,25)         131.0693      -DE/DX =    0.0            !
! A7    A(2,3,4)         118.2062      -DE/DX =    0.0            !
! A8    A(2,3,7)         120.8458      -DE/DX =    0.0            !
! A9    A(4,3,7)         120.9477      -DE/DX =    0.0            !
! A10   A(3,4,5)          120.9788      -DE/DX =    0.0            !
! A11   A(3,4,8)          119.4126      -DE/DX =    0.0            !
! A12   A(5,4,8)          119.6087      -DE/DX =    0.0            !
! A13   A(4,5,6)          120.9788      -DE/DX =    0.0            !
! A14   A(4,5,9)          119.6087      -DE/DX =    0.0            !
! A15   A(6,5,9)          119.4126      -DE/DX =    0.0            !
! A16   A(1,6,5)          118.2062      -DE/DX =    0.0            !
! A17   A(1,6,10)          120.8458      -DE/DX =    0.0            !
! A18   A(5,6,10)          120.9477      -DE/DX =    0.0            !
! A19   A(12,11,23)         127.4868      -DE/DX =    0.0            !
! A20   A(12,11,25)         127.4868      -DE/DX =    0.0            !
! A21   A(23,11,25)         105.0264      -DE/DX =    0.0            !
! A22   A(11,12,13)         121.1951      -DE/DX =    0.0            !
! A23   A(11,12,14)         121.1951      -DE/DX =    0.0            !
! A24   A(13,12,14)         117.6098      -DE/DX =    0.0            !
! A25   A(12,13,15)         121.405       -DE/DX =    0.0            !
! A26   A(12,13,16)         119.5475      -DE/DX =    0.0            !
! A27   A(15,13,16)         119.0421      -DE/DX =    0.0            !
! A28   A(12,14,17)         121.405       -DE/DX =    0.0            !
! A29   A(12,14,18)         119.5475      -DE/DX =    0.0            !
! A30   A(17,14,18)         119.0421      -DE/DX =    0.0            !
! A31   A(13,15,19)         119.9156      -DE/DX =    0.0            !
! A32   A(13,15,20)         120.0046      -DE/DX =    0.0            !
! A33   A(19,15,20)         120.0796      -DE/DX =    0.0            !
! A34   A(14,17,19)         119.9156      -DE/DX =    0.0            !
! A35   A(14,17,21)         120.0046      -DE/DX =    0.0            !
! A36   A(19,17,21)         120.0796      -DE/DX =    0.0            !
! A37   A(15,19,17)         119.7491      -DE/DX =    0.0            !
! A38   A(15,19,22)         120.1255      -DE/DX =    0.0            !
! A39   A(17,19,22)         120.1255      -DE/DX =    0.0            !
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! A40   A(1,23,11)          109.3695        -DE/DX =    0.0             !
! A41   A(1,23,24)          121.3143        -DE/DX =    0.0             !
! A42   A(11,23,24)         129.1947        -DE/DX =    0.0             !
! A43   A(2,25,11)          109.3695        -DE/DX =    0.0             !
! A44   A(2,25,26)          121.3143        -DE/DX =    0.0             !
! A45   A(11,25,26)         129.1947        -DE/DX =    0.0             !
! D1    D(6,1,2,3)           0.4751        -DE/DX =    0.0             !
! D2    D(6,1,2,25)       -179.5476        -DE/DX =    0.0             !
! D3    D(23,1,2,3)       -179.5479        -DE/DX =    0.0             !
! D4    D(23,1,2,25)         0.4294        -DE/DX =    0.0             !
! D5    D(2,1,6,5)          -0.3085        -DE/DX =    0.0             !
! D6    D(2,1,6,10)         179.8691        -DE/DX =    0.0             !
! D7    D(23,1,6,5)         179.7205        -DE/DX =    0.0             !
! D8    D(23,1,6,10)         -0.1019        -DE/DX =    0.0             !
! D9    D(2,1,23,11)         -0.348         -DE/DX =    0.0             !
! D10   D(2,1,23,24)       -176.6902        -DE/DX =    0.0             !
! D11   D(6,1,23,11)        179.6258        -DE/DX =    0.0             !
! D12   D(6,1,23,24)          3.2836        -DE/DX =    0.0             !
! D13   D(1,2,3,4)           -0.3084        -DE/DX =    0.0             !
! D14   D(1,2,3,7)          179.8692        -DE/DX =    0.0             !
! D15   D(25,2,3,4)         179.7203        -DE/DX =    0.0             !
! D16   D(25,2,3,7)          -0.1021        -DE/DX =    0.0             !
! D17   D(1,2,25,11)         -0.3489        -DE/DX =    0.0             !
! D18   D(1,2,25,26)       -176.6905        -DE/DX =    0.0             !
! D19   D(3,2,25,11)        179.6252        -DE/DX =    0.0             !
! D20   D(3,2,25,26)          3.2835        -DE/DX =    0.0             !
! D21   D(2,3,4,5)           -0.0056        -DE/DX =    0.0             !
! D22   D(2,3,4,8)         -179.9989        -DE/DX =    0.0             !
! D23   D(7,3,4,5)          179.8166        -DE/DX =    0.0             !
! D24   D(7,3,4,8)           -0.1767        -DE/DX =    0.0             !
! D25   D(3,4,5,6)            0.1649        -DE/DX =    0.0             !
! D26   D(3,4,5,9)         -179.8417        -DE/DX =    0.0             !
! D27   D(8,4,5,6)         -179.8419        -DE/DX =    0.0             !
! D28   D(8,4,5,9)            0.1515        -DE/DX =    0.0             !
! D29   D(4,5,6,1)           -0.0055        -DE/DX =    0.0             !
! D30   D(4,5,6,10)         179.8167        -DE/DX =    0.0             !
! D31   D(9,5,6,1)         -179.9989        -DE/DX =    0.0             !
! D32   D(9,5,6,10)          -0.1767        -DE/DX =    0.0             !
! D33   D(23,11,12,13)      -25.6974        -DE/DX =    0.0             !
! D34   D(23,11,12,14)      154.3026        -DE/DX =    0.0             !
! D35   D(25,11,12,13)      154.3033        -DE/DX =    0.0             !
! D36   D(25,11,12,14)      -25.6967        -DE/DX =    0.0             !
! D37   D(12,11,23,1)      -179.8661        -DE/DX =    0.0             !
! D38   D(12,11,23,24)       -3.8989        -DE/DX =    0.0             !
! D39   D(25,11,23,1)         0.1334        -DE/DX =    0.0             !
! D40   D(25,11,23,24)      176.1005        -DE/DX =    0.0             !
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 ! D41   D(12,11,25,2)       -179.8659       -DE/DX =    0.0              !
 ! D42   D(12,11,25,26)        -3.8993       -DE/DX =    0.0              !
 ! D43   D(23,11,25,2)          0.1347       -DE/DX =    0.0              !
 ! D44   D(23,11,25,26)       176.1013       -DE/DX =    0.0              !
 ! D45   D(11,12,13,15)      -179.9656       -DE/DX =    0.0              !
 ! D46   D(11,12,13,16)        -0.8179       -DE/DX =    0.0              !
 ! D47   D(14,12,13,15)         0.0344       -DE/DX =    0.0              !
 ! D48   D(14,12,13,16)       179.182        -DE/DX =    0.0              !
 ! D49   D(11,12,14,17)      -179.9657       -DE/DX =    0.0              !
 ! D50   D(11,12,14,18)        -0.818        -DE/DX =    0.0              !
 ! D51   D(13,12,14,17)         0.0343       -DE/DX =    0.0              !
 ! D52   D(13,12,14,18)       179.182        -DE/DX =    0.0              !
 ! D53   D(12,13,15,19)        -0.0686       -DE/DX =    0.0              !
 ! D54   D(12,13,15,20)       179.7891       -DE/DX =    0.0              !
 ! D55   D(16,13,15,19)      -179.2204       -DE/DX =    0.0              !
 ! D56   D(16,13,15,20)         0.6372       -DE/DX =    0.0              !
 ! D57   D(12,14,17,19)        -0.0685       -DE/DX =    0.0              !
 ! D58   D(12,14,17,21)       179.7891       -DE/DX =    0.0              !
 ! D59   D(18,14,17,19)      -179.2205       -DE/DX =    0.0              !
 ! D60   D(18,14,17,21)         0.6372       -DE/DX =    0.0              !
 ! D61   D(13,15,19,17)         0.0337       -DE/DX =    0.0              !
 ! D62   D(13,15,19,22)      -179.9663       -DE/DX =    0.0              !
 ! D63   D(20,15,19,17)      -179.8239       -DE/DX =    0.0              !
 ! D64   D(20,15,19,22)         0.1761       -DE/DX =    0.0              !
 ! D65   D(14,17,19,15)         0.0337       -DE/DX =    0.0              !
 ! D66   D(14,17,19,22)      -179.9663       -DE/DX =    0.0              !
 ! D67   D(21,17,19,15)      -179.8239       -DE/DX =    0.0              !
 ! D68   D(21,17,19,22)         0.1761       -DE/DX =    0.0              !
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 %mem=1GB
 %chk=T:\CHM\deg013\Thusini\Reproducing data of li et. al paper\-BDAB-1st
reactio
 n7-20\TPH-01-46-FREQ-BDAB-GAS PHASE.chk
 ----------------------------------------
 # freq wb97xd/6-31g(d,p) geom=connectivity
 ----------------------------------------
 1/10=4,30=1,38=1,57=2/1,3;
 2/12=2,17=6,18=5,40=1/2;
 3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
 4//1;
 5/5=2,38=5,98=1/2;
```

8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1/2;
6/7=2,8=2,9=2,10=2,18=1,28=1/1;
7/8=1,10=1,25=1/1,2,3,16;
1/10=4,30=1/3;
99//99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.91223	0.6964	0.11066
C	-1.91223	-0.69639	-0.11067
C	-3.10473	-1.39845	-0.22656
C	-4.30092	-0.68897	-0.11242
C	-4.30092	0.68897	0.11244
C	-3.10474	1.39845	0.22656
H	-3.10422	-2.47021	-0.39945
H	-5.24434	-1.21792	-0.20001
H	-5.24434	1.21791	0.20004
H	-3.10422	2.47021	0.39946
B	0.28106	0.	-0.00001
C	1.84079	0.	0.
C	2.56692	1.16502	-0.28689
C	2.56691	-1.16501	0.28689
C	3.95831	1.16959	-0.28875
H	2.03687	2.0842	-0.52423
C	3.9583	-1.16959	0.28876
H	2.03686	-2.08419	0.52422
C	4.65728	0.	0.00001
H	4.49756	2.08383	-0.51681
H	4.49755	-2.08384	0.51683
H	5.74296	-0.00001	0.00001
N	-0.59084	1.12465	0.17438
H	-0.36237	2.0847	0.36929
N	-0.59084	-1.12464	-0.17441
H	-0.36237	-2.08469	-0.36931

GradGradGradG

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.212362 (Hartree/Particle)
Thermal correction to Energy= 0.223545
Thermal correction to Enthalpy= 0.224489
Thermal correction to Gibbs Free Energy= 0.174265
Sum of electronic and zero-point Energies= -597.968336

Sum of electronic and thermal Energies= -597.957153
Sum of electronic and thermal Enthalpies= -597.956209
Sum of electronic and thermal Free Energies= -598.006433

Benzene1,2-diammine 3.2D

%nprocshared=2
Will use up to 2 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\Product\OPt-FREQ
-OPD-new-WB97XD-Gas phase.chk
---
opt freq wb97xd/6-31g(d,p)

1/14=-1,18=20,19=15,26=3,38=1/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4//1;
5/5=2,38=5/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(2);
2/9=110/2;
99//99;
2/9=110/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.92312	0.69619	0.01766
C	-0.71097	1.38794	0.0232
C	0.5078	0.70673	0.00108
C	0.5079	-0.70675	-0.00111
C	-0.71094	-1.38799	-0.02319
C	-1.92307	-0.69623	-0.01766
H	-2.8568	1.24659	0.03085
H	-0.70556	2.4737	0.03331
H	-0.70549	-2.47373	-0.0332
H	-2.85675	-1.24665	-0.03087
N	1.74385	-1.37998	-0.04596
H	2.4452	-0.97943	0.56751
H	1.6676	-2.37541	0.11784
N	1.74383	1.38012	0.04609
H	2.44504	0.97935	-0.56743
H	1.66732	2.37536	-0.1189

GradGradGradG

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! R8    R(4,5)              1.3915        -DE/DX =    0.0             !
! R9    R(4,11)             1.4062        -DE/DX =    0.0             !
! R10   R(5,6)              1.3937        -DE/DX =    0.0             !
! R11   R(5,9)              1.0873        -DE/DX =    0.0             !
! R12   R(6,10)             1.085         -DE/DX =    0.0             !
! R13   R(11,12)            1.0145        -DE/DX =    0.0             !
! R14   R(11,13)            1.0108        -DE/DX =    0.0             !
! R15   R(14,15)            1.0145        -DE/DX =    0.0             !
! R16   R(14,16)            1.0108        -DE/DX =    0.0             !
! A1    A(2,1,6)            119.798       -DE/DX =    0.0             !
! A2    A(2,1,7)            119.7585      -DE/DX =    0.0             !
! A3    A(6,1,7)            120.4391      -DE/DX =    0.0             !
! A4    A(1,2,3)            120.8408      -DE/DX =    0.0             !
! A5    A(1,2,8)            120.0712      -DE/DX =    0.0             !
! A6    A(3,2,8)            119.0855      -DE/DX =    0.0             !
! A7    A(2,3,4)            119.3464      -DE/DX =    0.0             !
! A8    A(2,3,14)           123.0649      -DE/DX =    0.0             !
! A9    A(4,3,14)           117.5431      -DE/DX =    0.0             !
! A10   A(3,4,5)            119.3463      -DE/DX =    0.0             !
! A11   A(3,4,11)           117.5431      -DE/DX =    0.0             !
! A12   A(5,4,11)           123.065       -DE/DX =    0.0             !
! A13   A(4,5,6)            120.8409      -DE/DX =    0.0             !
! A14   A(4,5,9)            119.0855      -DE/DX =    0.0             !
! A15   A(6,5,9)            120.0712      -DE/DX =    0.0             !
! A16   A(1,6,5)            119.7979      -DE/DX =    0.0             !
! A17   A(1,6,10)           120.4391      -DE/DX =    0.0             !
! A18   A(5,6,10)           119.7586      -DE/DX =    0.0             !
! A19   A(4,11,12)          111.7124      -DE/DX =    0.0             !
! A20   A(4,11,13)          112.9371      -DE/DX =    0.0             !
! A21   A(12,11,13)         110.1355      -DE/DX =    0.0             !
! A22   A(3,14,15)          111.711       -DE/DX =    0.0             !
! A23   A(3,14,16)          112.9366      -DE/DX =    0.0             !
! A24   A(15,14,16)         110.1349      -DE/DX =    0.0             !
! D1    D(6,1,2,3)          -0.5744       -DE/DX =    0.0             !
! D2    D(6,1,2,8)          178.8572      -DE/DX =    0.0             !
! D3    D(7,1,2,3)          -179.8169     -DE/DX =    0.0             !
! D4    D(7,1,2,8)          -0.3853       -DE/DX =    0.0             !
! D5    D(2,1,6,5)          1.3736        -DE/DX =    0.0             !
! D6    D(2,1,6,10)         -179.3894     -DE/DX =    0.0             !
! D7    D(7,1,6,5)          -179.3892     -DE/DX =    0.0             !
! D8    D(7,1,6,10)         -0.1521       -DE/DX =    0.0             !
! D9    D(1,2,3,4)          -1.0185       -DE/DX =    0.0             !
! D10   D(1,2,3,14)         -178.5016     -DE/DX =    0.0             !
! D11   D(8,2,3,4)          179.5444      -DE/DX =    0.0             !
! D12   D(8,2,3,14)         2.0613        -DE/DX =    0.0             !
! D13   D(2,3,4,5)          1.8006        -DE/DX =    0.0             !
```

```
 ! D14   D(2,3,4,11)         179.4219       -DE/DX =    0.0             !
 ! D15   D(14,3,4,5)         179.4218       -DE/DX =    0.0             !
 ! D16   D(14,3,4,11)         -2.9569       -DE/DX =    0.0             !
 ! D17   D(2,3,14,15)       -136.5994       -DE/DX =    0.0             !
 ! D18   D(2,3,14,16)        -11.7922       -DE/DX =    0.0             !
 ! D19   D(4,3,14,15)         45.8749       -DE/DX =    0.0             !
 ! D20   D(4,3,14,16)        170.6821       -DE/DX =    0.0             !
 ! D21   D(3,4,5,6)           -1.0179       -DE/DX =    0.0             !
 ! D22   D(3,4,5,9)          179.5447       -DE/DX =    0.0             !
 ! D23   D(11,4,5,6)        -178.5012       -DE/DX =    0.0             !
 ! D24   D(11,4,5,9)          2.0615       -DE/DX =    0.0             !
 ! D25   D(3,4,11,12)         45.8813       -DE/DX =    0.0             !
 ! D26   D(3,4,11,13)        170.6909       -DE/DX =    0.0             !
 ! D27   D(5,4,11,12)       -136.5928       -DE/DX =    0.0             !
 ! D28   D(5,4,11,13)        -11.7832       -DE/DX =    0.0             !
 ! D29   D(4,5,6,1)           -0.5749       -DE/DX =    0.0             !
 ! D30   D(4,5,6,10)        -179.8172       -DE/DX =    0.0             !
 ! D31   D(9,5,6,1)          178.8569       -DE/DX =    0.0             !
 ! D32   D(9,5,6,10)          -0.3854       -DE/DX =    0.0             !
 ---------------------------------------------------------------------------

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradG
radGrad

 ------------------
  - Thermochemistry -
  ------------------
  Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
Zero-point correction=                          0.136110 (Hartree/Particle)
  Thermal correction to Energy=                  0.143103
  Thermal correction to Enthalpy=                0.144047
  Thermal correction to Gibbs Free Energy=       0.105409
  Sum of electronic and zero-point Energies=          -342.724331
  Sum of electronic and thermal Energies=             -342.717338
  Sum of electronic and thermal Enthalpies=           -342.716394
  Sum of electronic and thermal Free Energies=        -342.755032
```

BDAB-W1 3.4D

```
******************************************
 %nprocshared=2
 Will use up to    2 processors via shared memory.
 %mem=1GB
 %chk=T:\CHM\deg013\Thusini\Reproducing data of li et. al paper\-BDAB-1st reactio
 n7-20\TPH-01-46-OPT-BDAB-W1-Gas phase.chk
 ---------------------------------------
 # opt wb97xd/6-31g(d,p) geom=connectivity
 ---------------------------------------
 1/14=-1,18=20,19=15,26=3,38=1,57=2/1,3;
 2/9=110,12=2,17=6,18=5,40=1/2;
 3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
 4//1;
 5/5=2,38=5/2;
 6/7=2,8=2,9=2,10=2,28=1/1;
 7//1,2,3,16;
 1/14=-1,18=20,19=15,26=3/3(2);
 2/9=110/2;
 99//99;
 2/9=110/2;
 3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
 4/5=5,16=3,69=1/1;
 5/5=2,38=5/2;
 7//1,2,3,16;
 1/14=-1,18=20,19=15,26=3/3(-5);
 2/9=110/2;
 6/7=2,8=2,9=2,10=2,19=2,28=1/1;
 99/9=1/99;
 ------------------
 Title Card Required
 ------------------
 Symbolic Z-matrix:
 Charge =  0 Multiplicity = 1
 C                 -1.90627  -0.74591   0.22979
 C                 -1.89673   0.59538   0.66213
 C                 -3.08144   1.27371   0.91322
 C                 -4.28279   0.5903    0.72297
 C                 -4.29342  -0.73839   0.29407
 C                 -3.10429  -1.42285   0.04207
 H                 -3.07138   2.30611   1.24848
 H                 -5.22153   1.10064   0.91151
 H                 -5.24079  -1.24849   0.154
 H                 -3.11288  -2.45539  -0.29247
 B                  0.29118  -0.07806   0.37986
```

C	1.85057	-0.06941	0.3556
C	2.56831	1.10821	0.10119
C	2.58264	-1.23754	0.61846
C	3.95968	1.12098	0.10177
H	2.03161	2.02932	-0.11205
C	3.97457	-1.23137	0.62598
H	2.05587	-2.16335	0.83542
C	4.66546	-0.05054	0.36558
H	4.49333	2.04394	-0.10241
H	4.51915	-2.14643	0.83664
H	5.75098	-0.04266	0.37015
N	-0.58887	-1.15753	0.05841
H	-0.36765	-2.0851	-0.26199
N	-0.56855	1.00655	0.76413
H	-0.33078	1.94483	1.04026
O	0.19596	0.01452	1.7434
H	1.15596	0.01452	1.7434
H	-0.12449	0.91946	1.7434

Add virtual bond connecting atoms H29 and N25 Dist= 2.04D+00.

GradGradGradG

```
! R6    R(3,4)              1.3946        -DE/DX =    0.0             !
! R7    R(3,7)              1.0857        -DE/DX =    0.0             !
! R8    R(4,5)              1.3955        -DE/DX =    0.0             !
! R9    R(4,8)              1.0849        -DE/DX =    0.0             !
! R10   R(5,6)               1.3944        -DE/DX =    0.0             !
! R11   R(5,9)               1.0849        -DE/DX =    0.0             !
! R12   R(6,10)              1.0855        -DE/DX =    0.0             !
! R13   R(11,12)              1.5597        -DE/DX =    0.0             !
! R14   R(11,23)              1.4288        -DE/DX =    0.0             !
! R15   R(11,25)              1.4353        -DE/DX =    0.0             !
! R16   R(12,13)              1.4018        -DE/DX =    0.0             !
! R17   R(12,14)              1.403         -DE/DX =    0.0             !
! R18   R(13,15)              1.391         -DE/DX =    0.0             !
! R19   R(13,16)              1.0874        -DE/DX =    0.0             !
! R20   R(14,17)              1.3916        -DE/DX =    0.0             !
! R21   R(14,18)              1.087         -DE/DX =    0.0             !
! R22   R(15,19)              1.3924        -DE/DX =    0.0             !
! R23   R(15,20)              1.0856        -DE/DX =    0.0             !
! R24   R(17,19)              1.3921        -DE/DX =    0.0             !
! R25   R(17,21)              1.0856        -DE/DX =    0.0             !
! R26   R(19,22)              1.0856        -DE/DX =    0.0             !
! R27   R(23,24)              1.0052        -DE/DX =    0.0             !
! R28   R(25,26)              1.0056        -DE/DX =    0.0             !
! R29   R(25,29)              2.6412        -DE/DX =    0.0             !
! R30   R(27,28)              0.9617        -DE/DX =    0.0             !
! R31   R(27,29)              0.9619        -DE/DX =    0.0             !
! A1    A(2,1,6)            120.716         -DE/DX =    0.0             !
! A2    A(2,1,23)            108.2008         -DE/DX =    0.0             !
! A3    A(6,1,23)            131.0831         -DE/DX =    0.0             !
! A4    A(1,2,3)            120.9851         -DE/DX =    0.0             !
! A5    A(1,2,25)            107.9766         -DE/DX =    0.0             !
! A6    A(3,2,25)            131.0356         -DE/DX =    0.0             !
! A7    A(2,3,4)            118.102         -DE/DX =    0.0             !
! A8    A(2,3,7)            120.9081         -DE/DX =    0.0             !
! A9    A(4,3,7)            120.9899         -DE/DX =    0.0             !
! A10   A(3,4,5)             120.9599         -DE/DX =    0.0             !
! A11   A(3,4,8)             119.3342         -DE/DX =    0.0             !
! A12   A(5,4,8)             119.7057         -DE/DX =    0.0             !
! A13   A(4,5,6)             121.0645         -DE/DX =    0.0             !
! A14   A(4,5,9)             119.6273         -DE/DX =    0.0             !
! A15   A(6,5,9)             119.3081         -DE/DX =    0.0             !
! A16   A(1,6,5)             118.1722         -DE/DX =    0.0             !
! A17   A(1,6,10)             120.8365         -DE/DX =    0.0             !
! A18   A(5,6,10)             120.9911         -DE/DX =    0.0             !
! A19   A(12,11,23)            128.1153         -DE/DX =    0.0             !
! A20   A(12,11,25)            126.7693         -DE/DX =    0.0             !
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! A21   A(23,11,25)        105.1073       -DE/DX =    0.0             !
! A22   A(11,12,13)        121.2492       -DE/DX =    0.0             !
! A23   A(11,12,14)        120.9184       -DE/DX =    0.0             !
! A24   A(13,12,14)        117.8244       -DE/DX =    0.0             !
! A25   A(12,13,15)        121.2775       -DE/DX =    0.0             !
! A26   A(12,13,16)        119.5233       -DE/DX =    0.0             !
! A27   A(15,13,16)        119.1934       -DE/DX =    0.0             !
! A28   A(12,14,17)        121.1977       -DE/DX =    0.0             !
! A29   A(12,14,18)        119.3489       -DE/DX =    0.0             !
! A30   A(17,14,18)        119.4315       -DE/DX =    0.0             !
! A31   A(13,15,19)        119.9243       -DE/DX =    0.0             !
! A32   A(13,15,20)        120.0085       -DE/DX =    0.0             !
! A33   A(19,15,20)        120.0672       -DE/DX =    0.0             !
! A34   A(14,17,19)        119.9541       -DE/DX =    0.0             !
! A35   A(14,17,21)        119.9376       -DE/DX =    0.0             !
! A36   A(19,17,21)        120.1079       -DE/DX =    0.0             !
! A37   A(15,19,17)        119.8207       -DE/DX =    0.0             !
! A38   A(15,19,22)        120.0756       -DE/DX =    0.0             !
! A39   A(17,19,22)        120.1034       -DE/DX =    0.0             !
! A40   A(1,23,11)         109.4777       -DE/DX =    0.0             !
! A41   A(1,23,24)         121.5521       -DE/DX =    0.0             !
! A42   A(11,23,24)        128.9611       -DE/DX =    0.0             !
! A43   A(2,25,11)         109.235        -DE/DX =    0.0             !
! A44   A(2,25,26)         121.4695       -DE/DX =    0.0             !
! A45   A(2,25,29)          92.3601       -DE/DX =    0.0             !
! A46   A(11,25,26)        129.2866       -DE/DX =    0.0             !
! A47   A(11,25,29)         74.6188       -DE/DX =    0.0             !
! A48   A(26,25,29)        102.71         -DE/DX =    0.0             !
! A49   A(28,27,29)        103.545        -DE/DX =    0.0             !
! A50   A(25,29,27)        137.6929       -DE/DX =    0.0             !
! D1    D(6,1,2,3)           0.0961      -DE/DX =    0.0             !
! D2    D(6,1,2,25)        179.566        -DE/DX =    0.0             !
! D3    D(23,1,2,3)       -180.001        -DE/DX =    0.0             !
! D4    D(23,1,2,25)        -0.531        -DE/DX =    0.0             !
! D5    D(2,1,6,5)          -0.0762       -DE/DX =    0.0             !
! D6    D(2,1,6,10)       -179.9271       -DE/DX =    0.0             !
! D7    D(23,1,6,5)       -179.9539       -DE/DX =    0.0             !
! D8    D(23,1,6,10)         0.1952       -DE/DX =    0.0             !
! D9    D(2,1,23,11)         0.3846       -DE/DX =    0.0             !
! D10   D(2,1,23,24)       179.3779       -DE/DX =    0.0             !
! D11   D(6,1,23,11)      -179.7261       -DE/DX =    0.0             !
! D12   D(6,1,23,24)        -0.7327       -DE/DX =    0.0             !
! D13   D(1,2,3,4)          -0.1038       -DE/DX =    0.0             !
! D14   D(1,2,3,7)         179.8849       -DE/DX =    0.0             !
! D15   D(25,2,3,4)       -179.4354       -DE/DX =    0.0             !
! D16   D(25,2,3,7)         0.5533       -DE/DX =    0.0             !
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! D17	D(1,2,25,11)	0.4777	-DE/DX = 0.0	!
! D18	D(1,2,25,26)	179.487	-DE/DX = 0.0	!
! D19	D(1,2,25,29)	-74.0496	-DE/DX = 0.0	!
! D20	D(3,2,25,11)	179.8753	-DE/DX = 0.0	!
! D21	D(3,2,25,26)	-1.1154	-DE/DX = 0.0	!
! D22	D(3,2,25,29)	105.348	-DE/DX = 0.0	!
! D23	D(2,3,4,5)	0.0971	-DE/DX = 0.0	!
! D24	D(2,3,4,8)	179.9678	-DE/DX = 0.0	!
! D25	D(7,3,4,5)	-179.8916	-DE/DX = 0.0	!
! D26	D(7,3,4,8)	-0.021	-DE/DX = 0.0	!
! D27	D(3,4,5,6)	-0.0823	-DE/DX = 0.0	!
! D28	D(3,4,5,9)	179.8252	-DE/DX = 0.0	!
! D29	D(8,4,5,6)	-179.9524	-DE/DX = 0.0	!
! D30	D(8,4,5,9)	-0.045	-DE/DX = 0.0	!
! D31	D(4,5,6,1)	0.0698	-DE/DX = 0.0	!
! D32	D(4,5,6,10)	179.9205	-DE/DX = 0.0	!
! D33	D(9,5,6,1)	-179.8379	-DE/DX = 0.0	!
! D34	D(9,5,6,10)	0.0128	-DE/DX = 0.0	!
! D35	D(23,11,12,13)	144.5227	-DE/DX = 0.0	!
! D36	D(23,11,12,14)	-36.5236	-DE/DX = 0.0	!
! D37	D(25,11,12,13)	-36.6704	-DE/DX = 0.0	!
! D38	D(25,11,12,14)	142.2832	-DE/DX = 0.0	!
! D39	D(12,11,23,1)	178.9185	-DE/DX = 0.0	!
! D40	D(12,11,23,24)	0.0217	-DE/DX = 0.0	!
! D41	D(25,11,23,1)	-0.0915	-DE/DX = 0.0	!
! D42	D(25,11,23,24)	-178.9884	-DE/DX = 0.0	!
! D43	D(12,11,25,2)	-179.2676	-DE/DX = 0.0	!
! D44	D(12,11,25,26)	1.8242	-DE/DX = 0.0	!
! D45	D(12,11,25,29)	-92.1766	-DE/DX = 0.0	!
! D46	D(23,11,25,2)	-0.2398	-DE/DX = 0.0	!
! D47	D(23,11,25,26)	-179.1481	-DE/DX = 0.0	!
! D48	D(23,11,25,29)	86.8511	-DE/DX = 0.0	!
! D49	D(11,12,13,15)	179.3452	-DE/DX = 0.0	!
! D50	D(11,12,13,16)	-1.5387	-DE/DX = 0.0	!
! D51	D(14,12,13,15)	0.3602	-DE/DX = 0.0	!
! D52	D(14,12,13,16)	179.4763	-DE/DX = 0.0	!
! D53	D(11,12,14,17)	-179.1034	-DE/DX = 0.0	!
! D54	D(11,12,14,18)	-0.8133	-DE/DX = 0.0	!
! D55	D(13,12,14,17)	-0.1149	-DE/DX = 0.0	!
! D56	D(13,12,14,18)	178.1752	-DE/DX = 0.0	!
! D57	D(12,13,15,19)	-0.3171	-DE/DX = 0.0	!
! D58	D(12,13,15,20)	179.6536	-DE/DX = 0.0	!
! D59	D(16,13,15,19)	-179.436	-DE/DX = 0.0	!
! D60	D(16,13,15,20)	0.5346	-DE/DX = 0.0	!
! D61	D(12,14,17,19)	-0.1727	-DE/DX = 0.0	!
! D62	D(12,14,17,21)	179.5992	-DE/DX = 0.0	!

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! D63   D(18,14,17,19)      -178.4614       -DE/DX =    0.0              !
! D64   D(18,14,17,21)       1.3105       -DE/DX =    0.0             !
! D65   D(13,15,19,17)       0.0199       -DE/DX =    0.0             !
! D66   D(13,15,19,22)      -179.8063       -DE/DX =    0.0              !
! D67   D(20,15,19,17)      -179.9508       -DE/DX =    0.0              !
! D68   D(20,15,19,22)       0.2231       -DE/DX =    0.0             !
! D69   D(14,17,19,15)       0.2213       -DE/DX =    0.0             !
! D70   D(14,17,19,22)      -179.9526       -DE/DX =    0.0              !
! D71   D(21,17,19,15)      -179.5502       -DE/DX =    0.0              !
! D72   D(21,17,19,22)       0.2759       -DE/DX =    0.0             !
! D73   D(2,25,29,27)       136.9917       -DE/DX =    0.0              !
! D74   D(11,25,29,27)       27.6845       -DE/DX =    0.0              !
! D75   D(26,25,29,27)      -99.9899       -DE/DX =    0.0              !
! D76   D(28,27,29,25)       34.5602       -DE/DX =    0.0              !
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GradGradGradG

C	1.95229	-0.70404	0.21348
C	3.13856	-1.26371	0.66636
C	4.33762	-0.67431	0.26671
C	4.34452	0.44752	-0.56325
C	3.15409	1.01226	-1.01956
H	3.13258	-2.13547	1.31349
H	5.27693	-1.09525	0.60948
H	5.28988	0.89038	-0.8586
H	3.16082	1.88567	-1.66408
B	-0.23889	-0.15286	-0.25477
C	-1.79853	-0.16587	-0.2632
C	-2.5158	-1.37026	-0.25202
C	-2.52947	1.03171	-0.26028
C	-3.90673	-1.38242	-0.24594
H	-1.9772	-2.3148	-0.26261
C	-3.921	1.02686	-0.24913
H	-1.99845	1.97992	-0.23857
C	-4.61187	-0.18174	-0.24427
H	-4.44143	-2.32722	-0.24298
H	-4.46599	1.96567	-0.24048
H	-5.69746	-0.18835	-0.23635
N	0.63903	0.76167	-0.91393
H	0.41076	1.55055	-1.49351
N	0.62406	-1.05915	0.44806
H	0.38556	-1.85144	1.0196
O	-0.41854	1.63891	2.26251
H	-1.24177	1.17254	2.09044
H	0.25633	0.97507	2.09204

GradGradGradG

Sum of electronic and thermal Free Energies= -674.396083

BDAB-INT-W1 3.8D

%nprocshared=2
Will use up to 2 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thusini\Reproducing data of li et. al paper\BDAB-product form
ation\TPH-01-46-OPT-BDAB-INT-1-W1-GAS PHASE-8-18.chk
---
opt wb97xd/6-31g(d,p) geom=connectivity

1/14=-1,18=20,19=15,26=3,38=1,57=2/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4//1;
5/5=2,38=5/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(2);
2/9=110/2;
99//99;
2/9=110/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.62648	-0.19284	-0.4741
C	-2.66431	0.72728	-0.27385
C	-3.92851	0.29704	0.10408
C	-4.16832	-1.06393	0.28505
C	-3.14164	-1.98202	0.10212
C	-1.87376	-1.54433	-0.27545
H	-4.7233	1.02208	0.26345

H	-5.15765	-1.39863	0.57777
H	-3.32353	-3.04085	0.2496
H	-1.05718	-2.24067	-0.43311
C	1.99351	0.27223	-0.04085
C	2.88473	0.5258	1.00861
C	2.44912	-0.50076	-1.11555
C	4.18436	0.03023	0.98826
H	2.54677	1.12387	1.85018
C	3.74829	-0.99752	-1.14641
H	1.768	-0.72198	-1.93255
C	4.61952	-0.73141	-0.09321
H	4.86119	0.2403	1.81098
H	4.08367	-1.59177	-1.99109
H	5.63255	-1.12269	-0.11225
B	0.51163	0.81781	0.00613
O	0.06684	1.38886	1.18313
H	-0.84052	1.69815	1.10755
O	0.61884	2.08143	-0.88509
H	-0.16941	1.80744	-1.3736
H	0.33293	2.83557	-0.35764
N	-0.41819	0.24634	-0.91772
N	-2.30852	2.14572	-0.42328
H	-2.60608	2.47126	-1.32077
H	-2.76007	2.67973	0.29153
H	-0.03825	-0.65492	-0.70946

Add virtual bond connecting atoms O25 and B22 Dist= 2.93D+00.
Add virtual bond connecting atoms H26 and N28 Dist= 3.11D+00.

GradGradGradG

Name	Definition	Value	Derivative Info.
R1	R(1,2)	1.4083	-DE/DX = 0.0
R2	R(1,6)	1.3961	-DE/DX = 0.0
R3	R(1,28)	1.4131	-DE/DX = 0.0
R4	R(2,3)	1.3965	-DE/DX = 0.0
R5	R(2,29)	1.4086	-DE/DX = 0.0
R6	R(3,4)	1.3888	-DE/DX = 0.0
R7	R(3,7)	1.0871	-DE/DX = 0.0
R8	R(4,5)	1.3899	-DE/DX = 0.0
R9	R(4,8)	1.0849	-DE/DX = 0.0
R10	R(5,6)	1.389	-DE/DX = 0.0
R11	R(5,9)	1.0845	-DE/DX = 0.0
R12	R(6,10)	1.087	-DE/DX = 0.0
R13	R(11,12)	1.4022	-DE/DX = 0.0
R14	R(11,13)	1.4022	-DE/DX = 0.0
R15	R(11,22)	1.5777	-DE/DX = 0.0
R16	R(12,14)	1.3906	-DE/DX = 0.0
R17	R(12,15)	1.0861	-DE/DX = 0.0
R18	R(13,16)	1.392	-DE/DX = 0.0
R19	R(13,17)	1.0884	-DE/DX = 0.0
R20	R(14,18)	1.3929	-DE/DX = 0.0
R21	R(14,19)	1.0857	-DE/DX = 0.0
R22	R(16,18)	1.3916	-DE/DX = 0.0
R23	R(16,20)	1.0857	-DE/DX = 0.0
R24	R(18,21)	1.0857	-DE/DX = 0.0
R25	R(22,23)	1.3688	-DE/DX = 0.0
R26	R(22,25)	2.9927	-DE/DX = 0.0
R27	R(22,28)	1.4284	-DE/DX = 0.0
R28	R(23,24)	0.9757	-DE/DX = 0.0
R29	R(25,26)	0.9666	-DE/DX = 0.0
R30	R(25,27)	0.962	-DE/DX = 0.0
R31	R(26,28)	3.4234	-DE/DX = 0.0
R32	R(28,32)	1.01	-DE/DX = 0.0
R33	R(29,30)	1.0225	-DE/DX = 0.0
R34	R(29,31)	1.0112	-DE/DX = 0.0
A1	A(2,1,6)	118.8175	-DE/DX = 0.0
A2	A(2,1,28)	122.0503	-DE/DX = 0.0
A3	A(6,1,28)	119.1084	-DE/DX = 0.0
A4	A(1,2,3)	118.9643	-DE/DX = 0.0
A5	A(1,2,29)	120.1782	-DE/DX = 0.0
A6	A(3,2,29)	120.7843	-DE/DX = 0.0
A7	A(2,3,4)	121.4729	-DE/DX = 0.0
A8	A(2,3,7)	118.609	-DE/DX = 0.0
A9	A(4,3,7)	119.9104	-DE/DX = 0.0

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! A10   A(3,4,5)          119.6384       -DE/DX =    0.0             !
! A11   A(3,4,8)          119.7622       -DE/DX =    0.0             !
! A12   A(5,4,8)          120.5965       -DE/DX =    0.0             !
! A13   A(4,5,6)          119.37         -DE/DX =    0.0             !
! A14   A(4,5,9)          120.7266       -DE/DX =    0.0             !
! A15   A(6,5,9)          119.8981       -DE/DX =    0.0             !
! A16   A(1,6,5)          121.6922       -DE/DX =    0.0             !
! A17   A(1,6,10)         118.4556       -DE/DX =    0.0             !
! A18   A(5,6,10)         119.8403       -DE/DX =    0.0             !
! A19   A(12,11,13)       117.5993       -DE/DX =    0.0             !
! A20   A(12,11,22)       119.6665       -DE/DX =    0.0             !
! A21   A(13,11,22)       122.697        -DE/DX =    0.0             !
! A22   A(11,12,14)       121.3175       -DE/DX =    0.0             !
! A23   A(11,12,15)       118.842        -DE/DX =    0.0             !
! A24   A(14,12,15)       119.8404       -DE/DX =    0.0             !
! A25   A(11,13,16)       121.4887       -DE/DX =    0.0             !
! A26   A(11,13,17)       119.874        -DE/DX =    0.0             !
! A27   A(16,13,17)       118.6258       -DE/DX =    0.0             !
! A28   A(12,14,18)       120.0063       -DE/DX =    0.0             !
! A29   A(12,14,19)       120.0102       -DE/DX =    0.0             !
! A30   A(18,14,19)       119.983        -DE/DX =    0.0             !
! A31   A(13,16,18)       119.7986       -DE/DX =    0.0             !
! A32   A(13,16,20)       120.0735       -DE/DX =    0.0             !
! A33   A(18,16,20)       120.1272       -DE/DX =    0.0             !
! A34   A(14,18,16)       119.7823       -DE/DX =    0.0             !
! A35   A(14,18,21)       120.1221       -DE/DX =    0.0             !
! A36   A(16,18,21)       120.0939       -DE/DX =    0.0             !
! A37   A(11,22,23)       116.6686       -DE/DX =    0.0             !
! A38   A(11,22,25)        91.5772       -DE/DX =    0.0             !
! A39   A(11,22,28)       118.6243       -DE/DX =    0.0             !
! A40   A(23,22,25)        74.3324       -DE/DX =    0.0             !
! A41   A(23,22,28)       124.6726       -DE/DX =    0.0             !
! A42   A(25,22,28)       102.119        -DE/DX =    0.0             !
! A43   A(22,23,24)       111.9475       -DE/DX =    0.0             !
! A44   A(22,25,26)        52.6217       -DE/DX =    0.0             !
! A45   A(22,25,27)        74.428        -DE/DX =    0.0             !
! A46   A(26,25,27)       103.1773       -DE/DX =    0.0             !
! A47   A(25,26,28)        91.1897       -DE/DX =    0.0             !
! A48   A(1,28,22)        132.1393       -DE/DX =    0.0             !
! A49   A(1,28,26)        112.8032       -DE/DX =    0.0             !
! A50   A(1,28,32)        111.7348       -DE/DX =    0.0             !
! A51   A(22,28,26)        40.9942       -DE/DX =    0.0             !
! A52   A(22,28,32)       114.3086       -DE/DX =    0.0             !
! A53   A(26,28,32)       128.2578       -DE/DX =    0.0             !
! A54   A(2,29,30)        114.7892       -DE/DX =    0.0             !
! A55   A(2,29,31)        112.5007       -DE/DX =    0.0             !
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! A56   A(30,29,31)        109.6434       -DE/DX =    0.0             !
! D1    D(6,1,2,3)          2.4248       -DE/DX =    0.0            !
! D2    D(6,1,2,29)       179.3356        -DE/DX =    0.0             !
! D3    D(28,1,2,3)      -179.3639        -DE/DX =    0.0             !
! D4    D(28,1,2,29)       -2.4531        -DE/DX =    0.0            !
! D5    D(2,1,6,5)         -1.539        -DE/DX =    0.0            !
! D6    D(2,1,6,10)       179.7172        -DE/DX =    0.0             !
! D7    D(28,1,6,5)      -179.8038        -DE/DX =    0.0             !
! D8    D(28,1,6,10)        1.4524        -DE/DX =    0.0            !
! D9    D(2,1,28,22)       44.6276        -DE/DX =    0.0             !
! D10   D(2,1,28,26)        0.9946        -DE/DX =    0.0             !
! D11   D(2,1,28,32)     -151.9683         -DE/DX =    0.0             !
! D12   D(6,1,28,22)     -137.1661         -DE/DX =    0.0             !
! D13   D(6,1,28,26)      179.2009         -DE/DX =    0.0             !
! D14   D(6,1,28,32)       26.238         -DE/DX =    0.0            !
! D15   D(1,2,3,4)         -1.5401        -DE/DX =    0.0            !
! D16   D(1,2,3,7)        179.4722        -DE/DX =    0.0             !
! D17   D(29,2,3,4)       -178.4316         -DE/DX =    0.0             !
! D18   D(29,2,3,7)         2.5807        -DE/DX =    0.0            !
! D19   D(1,2,29,30)       46.2989         -DE/DX =    0.0             !
! D20   D(1,2,29,31)      172.6052         -DE/DX =    0.0             !
! D21   D(3,2,29,30)     -136.8472         -DE/DX =    0.0             !
! D22   D(3,2,29,31)      -10.5409         -DE/DX =    0.0             !
! D23   D(2,3,4,5)         -0.315         -DE/DX =    0.0            !
! D24   D(2,3,4,8)       -179.6945         -DE/DX =    0.0             !
! D25   D(7,3,4,5)        178.6597         -DE/DX =    0.0             !
! D26   D(7,3,4,8)         -0.7197        -DE/DX =    0.0            !
! D27   D(3,4,5,6)          1.2451        -DE/DX =    0.0            !
! D28   D(3,4,5,9)       -179.5878         -DE/DX =    0.0             !
! D29   D(8,4,5,6)       -179.3808         -DE/DX =    0.0             !
! D30   D(8,4,5,9)         -0.2136        -DE/DX =    0.0            !
! D31   D(4,5,6,1)         -0.3113        -DE/DX =    0.0            !
! D32   D(4,5,6,10)       178.4155         -DE/DX =    0.0             !
! D33   D(9,5,6,1)        -179.4854         -DE/DX =    0.0             !
! D34   D(9,5,6,10)        -0.7586        -DE/DX =    0.0            !
! D35   D(13,11,12,14)      -0.9862         -DE/DX =    0.0             !
! D36   D(13,11,12,15)     178.9506          -DE/DX =    0.0              !
! D37   D(22,11,12,14)    -178.8295          -DE/DX =    0.0              !
! D38   D(22,11,12,15)      1.1073         -DE/DX =    0.0             !
! D39   D(12,11,13,16)      0.5465         -DE/DX =    0.0             !
! D40   D(12,11,13,17)    -178.2024          -DE/DX =    0.0              !
! D41   D(22,11,13,16)     178.3196          -DE/DX =    0.0              !
! D42   D(22,11,13,17)      -0.4292         -DE/DX =    0.0             !
! D43   D(12,11,22,23)      23.4847         -DE/DX =    0.0             !
! D44   D(12,11,22,25)      96.7171         -DE/DX =    0.0             !
! D45   D(12,11,22,28)    -158.5512          -DE/DX =    0.0              !
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 ! D46   D(13,11,22,23)     -154.2441      -DE/DX =    0.0             !
 ! D47   D(13,11,22,25)      -81.0116      -DE/DX =    0.0             !
 ! D48   D(13,11,22,28)       23.72        -DE/DX =    0.0             !
 ! D49   D(11,12,14,18)       0.7175       -DE/DX =    0.0             !
 ! D50   D(11,12,14,19)     -179.533       -DE/DX =    0.0             !
 ! D51   D(15,12,14,18)     -179.2187      -DE/DX =    0.0             !
 ! D52   D(15,12,14,19)       0.5308       -DE/DX =    0.0             !
 ! D53   D(11,13,16,18)       0.162        -DE/DX =    0.0             !
 ! D54   D(11,13,16,20)     -179.5465      -DE/DX =    0.0             !
 ! D55   D(17,13,16,18)      178.926       -DE/DX =    0.0             !
 ! D56   D(17,13,16,20)       -0.7825      -DE/DX =    0.0             !
 ! D57   D(12,14,18,16)        0.0219      -DE/DX =    0.0             !
 ! D58   D(12,14,18,21)      179.5653      -DE/DX =    0.0             !
 ! D59   D(19,14,18,16)     -179.7277      -DE/DX =    0.0             !
 ! D60   D(19,14,18,21)       -0.1843      -DE/DX =    0.0             !
 ! D61   D(13,16,18,14)       -0.4538      -DE/DX =    0.0             !
 ! D62   D(13,16,18,21)     -179.9974      -DE/DX =    0.0             !
 ! D63   D(20,16,18,14)      179.2545      -DE/DX =    0.0             !
 ! D64   D(20,16,18,21)       -0.289       -DE/DX =    0.0             !
 ! D65   D(11,22,23,24)      164.1733      -DE/DX =    0.0             !
 ! D66   D(25,22,23,24)       80.4242      -DE/DX =    0.0             !
 ! D67   D(28,22,23,24)      -13.6537      -DE/DX =    0.0             !
 ! D68   D(11,22,25,26)      -90.2442      -DE/DX =    0.0             !
 ! D69   D(11,22,25,27)       30.4667      -DE/DX =    0.0             !
 ! D70   D(23,22,25,26)       27.0528      -DE/DX =    0.0             !
 ! D71   D(23,22,25,27)      147.7637      -DE/DX =    0.0             !
 ! D72   D(28,22,25,26)      150.0146      -DE/DX =    0.0             !
 ! D73   D(28,22,25,27)      -89.2745      -DE/DX =    0.0             !
 ! D74   D(11,22,28,1)       175.715       -DE/DX =    0.0             !
 ! D75   D(11,22,28,26)     -108.4262      -DE/DX =    0.0             !
 ! D76   D(11,22,28,32)       12.6403      -DE/DX =    0.0             !
 ! D77   D(23,22,28,1)        -6.4973      -DE/DX =    0.0             !
 ! D78   D(23,22,28,26)       69.3615      -DE/DX =    0.0             !
 ! D79   D(23,22,28,32)     -169.572       -DE/DX =    0.0             !
 ! D80   D(25,22,28,1)       -85.7008      -DE/DX =    0.0             !
 ! D81   D(25,22,28,26)       -9.842       -DE/DX =    0.0             !
 ! D82   D(25,22,28,32)      111.2245      -DE/DX =    0.0             !
 ! D83   D(22,25,26,28)      -11.7664      -DE/DX =    0.0             !
 ! D84   D(27,25,26,28)      -70.0427      -DE/DX =    0.0             !
 ! D85   D(25,26,28,1)       -82.4308      -DE/DX =    0.0             !
 ! D86   D(25,26,28,22)      148.8307      -DE/DX =    0.0             !
 ! D87   D(25,26,28,32)       65.0393      -DE/DX =    0.0             !
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 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradG
 radGrad
```

%nprocshared=2
Will use up to 2 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thusini\Reproducing data of li et. al paper\BDAB-product form
ation\TPH-01-46-FREQ-BDAB-INT-1-W1-GAS PHASE-8-18.chk
---
freq wb97xd/6-31g(d,p) geom=connectivity

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.265326 (Hartree/Particle)
Thermal correction to Energy= 0.281545
Thermal correction to Enthalpy= 0.282489
Thermal correction to Gibbs Free Energy= 0.221140
Sum of electronic and zero-point Energies= -750.751924
Sum of electronic and thermal Energies= -750.735704
Sum of electronic and thermal Enthalpies= -750.734760
Sum of electronic and thermal Free Energies= -750.796110

TS1-D

%mem=5GB
%chk=T:\CHM\deg013\Thusini\Reproducing data of li et. al paper\TPH-01-46\TPH-01-
46-QST3-BDAB-W1.chk
---
opt=(calcall,qst3,noeigentest) wb97xd/6-31g(d,p) geom=connectivity
---
1/5=1,10=4,11=1,14=-1,18=20,26=3,27=203,38=1,57=2/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
4//1;
5/5=2,38=5/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1/2;
6/7=2,8=2,9=2,10=2,18=1,28=1/1;
7/10=1,25=1/1,2,3,16;
1/5=1,10=4,11=1,14=-1,18=20,26=3,27=203/3(3);
2/9=110/2;
7/8=1,9=1,25=1,44=-1/16;
99//99;

```
2/9=110/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1/2;
7/10=1,25=1/1,2,3,16;
1/5=1,10=4,11=1,14=-1,18=20,26=3,27=203/3(-8);
2/9=110/2;
6/7=2,8=2,9=2,10=2,18=1,19=2,28=1/1;
7/8=1,9=1,25=1,44=-1/16;
99//99;
------------------
Title Card Required
------------------
Symbolic Z-matrix:
Charge =  0 Multiplicity = 1
C                  1.97149   0.63903  -0.44861
C                  1.96196  -0.70226  -0.01627
C                  3.14666  -1.38059   0.23482
C                  4.34801  -0.69718   0.04457
C                  4.35865   0.63151  -0.38433
C                  3.16952   1.31597  -0.63633
H                  3.1366   -2.41299   0.57009
H                  5.28676  -1.20751   0.23311
H                  5.30601   1.14161  -0.5244
H                  3.1781    2.34852  -0.97087
B                 -0.22595  -0.02881  -0.29854
C                 -1.78535  -0.03747  -0.3228
C                 -2.50308  -1.21509  -0.5772
C                 -2.51742   1.13066  -0.05994
C                 -3.89445  -1.22786  -0.57663
H                 -1.96639  -2.1362   -0.79045
C                 -3.90934   1.12449  -0.05241
H                 -1.99064   2.05647   0.15702
C                 -4.60024  -0.05633  -0.31282
H                 -4.42811  -2.15082  -0.78081
H                 -4.45392   2.03956   0.15825
H                 -5.68576  -0.06422  -0.30825
N                  0.65409   1.05065  -0.61999
H                  0.43287   1.97823  -0.94039
N                  0.63377  -1.11343   0.08573
H                  0.39601  -2.0517    0.36186
O                 -0.52644   0.46179   2.7616
H                 -0.21604   1.23875   3.23233
```

H -0.751 -0.2261 3.39246

Add virtual bond connecting atoms O27 and B11 Dist= 5.88D+00.

Title Card Required

Item	Value	Threshold	Converged?
Maximum Force	0.000002	0.000450	YES
RMS Force	0.000001	0.000300	YES
Maximum Displacement	0.001254	0.001800	YES
RMS Displacement	0.000280	0.001200	YES

Predicted change in Energy=-1.876933D-09

Optimization completed.

-- Stationary point found.

! Optimized Parameters !
! (Angstroms and Degrees) !

! Name	Definition	TS	Reactant	Product	Derivative Info.
! R1	R(1,2)	1.407	1.4093	1.4044	-DE/DX = 0.0 !
! R2	R(1,6)	1.3916	1.3888	1.4019	-DE/DX = 0.0 !
! R3	R(1,23)	1.381	1.3908	1.3623	-DE/DX = 0.0 !
! R4	R(2,3)	1.3794	1.3881	1.379	-DE/DX = 0.0 !
! R5	R(2,25)	1.4316	1.3941	1.4554	-DE/DX = 0.0 !
! R6	R(3,4)	1.3995	1.3952	1.3972	-DE/DX = 0.0 !
! R7	R(3,7)	1.0861	1.0855	1.0862	-DE/DX = 0.0 !
! R8	R(4,5)	1.391	1.3962	1.3954	-DE/DX = 0.0 !
! R9	R(4,8)	1.0845	1.085	1.084	-DE/DX = 0.0 !
! R10	R(5,6)	1.3968	1.395	1.3923	-DE/DX = 0.0 !
! R11	R(5,9)	1.0857	1.085	1.0861	-DE/DX = 0.0 !
! R12	R(6,10)	1.0857	1.0854	1.0853	-DE/DX = 0.0 !
! R13	R(11,12)	1.5935	1.5596	1.6163	-DE/DX = 0.0 !
! R14	R(11,23)	1.48	1.4294	1.5295	-DE/DX = 0.0 !
! R15	R(11,25)	1.5923	1.4364	1.7208	-DE/DX = 0.0 !
! R16	R(11,27)	1.6415	3.1137	1.433	-DE/DX = 0.0 !
! R17	R(12,13)	1.4025	1.4024	1.4034	-DE/DX = 0.0 !
! R18	R(12,14)	1.4001	1.4034	1.4004	-DE/DX = 0.0 !
! R19	R(13,15)	1.3917	1.3914	1.3928	-DE/DX = 0.0 !
! R20	R(13,16)	1.0901	1.0872	1.0897	-DE/DX = 0.0 !
! R21	R(14,17)	1.3917	1.392	1.3932	-DE/DX = 0.0 !
! R22	R(14,18)	1.0867	1.0871	1.0871	-DE/DX = 0.0 !
! R23	R(15,19)	1.392	1.3929	1.3927	-DE/DX = 0.0 !
! R24	R(15,20)	1.086	1.0855	1.0862	-DE/DX = 0.0 !
! R25	R(17,19)	1.3918	1.3927	1.3927	-DE/DX = 0.0 !
! R26	R(17,21)	1.0859	1.0855	1.0863	-DE/DX = 0.0 !

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! R27   R(19,22)         1.0856   1.0856   1.0859 -DE/DX =   0.0        !
! R28   R(23,24)         1.0048   1.006    1.007  -DE/DX =   0.0        !
! R29   R(25,26)         1.0132   1.0065   1.0181 -DE/DX =   0.0        !
! R30   R(25,29)         1.3317   3.6932   1.0191 -DE/DX =   0.0        !
! R31   R(27,28)         0.9629   0.96     0.9582 -DE/DX =   0.0        !
! R32   R(27,29)         1.1876   0.96     2.4448 -DE/DX =   0.0        !
! A1    A(2,1,6)        119.4298  120.745  117.9192 -DE/DX =   0.0        !
! A2    A(2,1,23)       110.6237  108.2446 112.571  -DE/DX =   0.0        !
! A3    A(6,1,23)       129.9321  131.0101 129.5057 -DE/DX =   0.0        !
! A4    A(1,2,3)        121.829   120.9863 123.2333 -DE/DX =   0.0        !
! A5    A(1,2,25)       109.661   108.035  109.6174 -DE/DX =   0.0        !
! A6    A(3,2,25)       128.4893  130.9782 127.1468 -DE/DX =   0.0        !
! A7    A(2,3,4)        118.5885  118.0918 118.3959 -DE/DX =   0.0        !
! A8    A(2,3,7)        120.5137  120.846  120.5816 -DE/DX =   0.0        !
! A9    A(4,3,7)        120.8969  121.0623 121.0221 -DE/DX =   0.0        !
! A10   A(3,4,5)        119.9747  120.9699 119.3574 -DE/DX =   0.0        !
! A11   A(3,4,8)        119.8494  119.4006 120.1491 -DE/DX =   0.0        !
! A12   A(5,4,8)        120.1736  119.6294 120.4934 -DE/DX =   0.0        !
! A13   A(4,5,6)        121.4292  121.0585 121.9765 -DE/DX =   0.0        !
! A14   A(4,5,9)        119.5148  119.5824 119.2194 -DE/DX =   0.0        !
! A15   A(6,5,9)        119.056   119.359  118.804  -DE/DX =   0.0        !
! A16   A(1,6,5)        118.7327  118.1484 119.1144 -DE/DX =   0.0        !
! A17   A(1,6,10)       120.5323  120.8084 120.1695 -DE/DX =   0.0        !
! A18   A(5,6,10)       120.7305  121.0431 120.7161 -DE/DX =   0.0        !
! A19   A(12,11,23)     120.8093  128.0465 115.7889 -DE/DX =   0.0        !
! A20   A(12,11,25)     119.202   126.7573 107.2688 -DE/DX =   0.0        !
! A21   A(12,11,27)     110.7175   85.3926 115.4402 -DE/DX =   0.0        !
! A22   A(23,11,25)     101.3483  105.1837  96.0063 -DE/DX =   0.0        !
! A23   A(23,11,27)     111.6516   99.2907 113.9494 -DE/DX =   0.0        !
! A24   A(25,11,27)      88.4025   85.0557 105.6339 -DE/DX =   0.0        !
! A25   A(11,12,13)     122.61    121.2791 121.2792 -DE/DX =   0.0        !
! A26   A(11,12,14)     120.2292  120.933  121.7015 -DE/DX =   0.0        !
! A27   A(13,12,14)     117.1256  117.7725 116.9933 -DE/DX =   0.0        !
! A28   A(12,13,15)     121.8127  121.2924 121.904  -DE/DX =   0.0        !
! A29   A(12,13,16)     120.1012  119.6298 119.6473 -DE/DX =   0.0        !
! A30   A(15,13,16)     118.0821  119.0743 118.4477 -DE/DX =   0.0        !
! A31   A(12,14,17)     121.6325  121.2618 121.7365 -DE/DX =   0.0        !
! A32   A(12,14,18)     118.7444  119.5705 118.6041 -DE/DX =   0.0        !
! A33   A(17,14,18)     119.6201  119.1612 119.6593 -DE/DX =   0.0        !
! A34   A(13,15,19)     119.8238  119.9361 119.8235 -DE/DX =   0.0        !
! A35   A(13,15,20)     120.1223  119.9548 120.0748 -DE/DX =   0.0        !
! A36   A(19,15,20)     120.0539  120.109  120.1016 -DE/DX =   0.0        !
! A37   A(14,17,19)     120.0658  119.9227 120.0441 -DE/DX =   0.0        !
! A38   A(14,17,21)     119.9165  119.9334 120.0395 -DE/DX =   0.0        !
! A39   A(19,17,21)     120.0172  120.1437 119.9163 -DE/DX =   0.0        !
! A40   A(15,19,17)     119.5334  119.8134 119.4965 -DE/DX =   0.0        !
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! A41   A(15,19,22)     120.1459  120.0903  120.2536 -DE/DX =    0.0         !
! A42   A(17,19,22)     120.3203  120.0962  120.2497 -DE/DX =    0.0         !
! A43   A(1,23,11)      111.5353  109.3886  114.5703 -DE/DX =    0.0         !
! A44   A(1,23,24)      120.1619  121.3615  118.4973 -DE/DX =    0.0         !
! A45   A(11,23,24)     127.0231  129.2413  122.9002 -DE/DX =    0.0         !
! A46   A(2,25,11)      106.502   109.1445  106.2941 -DE/DX =    0.0         !
! A47   A(2,25,26)      115.3429  121.3355  112.2051 -DE/DX =    0.0         !
! A48   A(2,25,29)      116.5529  110.6019  112.2718 -DE/DX =    0.0         !
! A49   A(11,25,26)     119.3623  129.4864  111.3494 -DE/DX =    0.0         !
! A50   A(26,25,29)     119.6513   83.6713  107.8658 -DE/DX =    0.0         !
! A51   A(11,27,28)     113.4519  125.3253  111.0155 -DE/DX =    0.0         !
! A52   A(11,27,29)      72.8145  123.7455   64.472  -DE/DX =    0.0         !
! A53   A(28,27,29)     115.9886  109.4712  121.0741 -DE/DX =    0.0         !
! D1    D(6,1,2,3)       -1.3088    0.0942   -0.5877 -DE/DX =    0.0         !
! D2    D(6,1,2,25)     177.1701  179.8636  178.8765 -DE/DX =    0.0         !
! D3    D(23,1,2,3)     177.4417  179.8888  178.7427 -DE/DX =    0.0         !
! D4    D(23,1,2,25)     -4.0794   -0.3417   -1.7931 -DE/DX =    0.0         !
! D5    D(2,1,6,5)        1.2754   -0.039     0.5471 -DE/DX =    0.0         !
! D6    D(2,1,6,10)    -179.4912  179.898  -179.5091 -DE/DX =    0.0         !
! D7    D(23,1,6,5)    -177.1996 -179.7805 -178.6516 -DE/DX =    0.0         !
! D8    D(23,1,6,10)      2.0338    0.1564    1.2923 -DE/DX =    0.0         !
! D9    D(2,1,23,11)      6.1497   -0.0375    8.3184 -DE/DX =    0.0         !
! D10   D(2,1,23,24)    174.1133 -179.0651  166.415  -DE/DX =    0.0         !
! D11   D(6,1,23,11)   -175.2695  179.7286 -172.4484 -DE/DX =    0.0         !
! D12   D(6,1,23,24)     -7.3059    0.701   -14.3518 -DE/DX =    0.0         !
! D13   D(1,2,3,4)        0.3238   -0.1149    0.1611 -DE/DX =    0.0         !
! D14   D(1,2,3,7)      179.9787  179.8501  179.9343 -DE/DX =    0.0         !
! D15   D(25,2,3,4)    -177.8461 -179.8245 -179.2057 -DE/DX =    0.0         !
! D16   D(25,2,3,7)       1.8088    0.1405    0.5675 -DE/DX =    0.0         !
! D17   D(1,2,25,11)      0.5745    0.5897   -4.4053 -DE/DX =    0.0         !
! D18   D(1,2,25,26)    135.4978  178.6693  117.532  -DE/DX =    0.0         !
! D19   D(1,2,25,29)    -76.4393  -86.1094 -120.7825 -DE/DX =    0.0         !
! D20   D(3,2,25,11)    178.9233 -179.6721  175.0324 -DE/DX =    0.0         !
! D21   D(3,2,25,26)    -46.1534   -1.5925  -63.0303 -DE/DX =    0.0         !
! D22   D(3,2,25,29)    101.9096   93.6288   58.6552 -DE/DX =    0.0         !
! D23   D(2,3,4,5)        0.6601    0.0852    0.2968 -DE/DX =    0.0         !
! D24   D(2,3,4,8)     -179.8785 -179.9073 -179.824  -DE/DX =    0.0         !
! D25   D(7,3,4,5)     -178.9934 -179.8797 -179.4754 -DE/DX =    0.0         !
! D26   D(7,3,4,8)        0.468     0.1278    0.4038 -DE/DX =    0.0         !
! D27   D(3,4,5,6)       -0.6718   -0.0336   -0.324  -DE/DX =    0.0         !
! D28   D(3,4,5,9)      179.3745  179.9626  179.6502 -DE/DX =    0.0         !
! D29   D(8,4,5,6)      179.8685  179.959   179.7973 -DE/DX =    0.0         !
! D30   D(8,4,5,9)       -0.0851   -0.0448   -0.2285 -DE/DX =    0.0         !
! D31   D(4,5,6,1)       -0.3135    0.0095   -0.1109 -DE/DX =    0.0         !
! D32   D(4,5,6,10)    -179.5453 -179.9273  179.9455 -DE/DX =    0.0         !
! D33   D(9,5,6,1)      179.6404 -179.9868  179.9148 -DE/DX =    0.0         !
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! D34   D(9,5,6,10)       0.4086    0.0764   -0.0288 -DE/DX =    0.0         !
! D35   D(23,11,12,13)  -172.233   150.9728 -175.3755 -DE/DX =    0.0         !
! D36   D(23,11,12,14)    9.9879  -30.4867    6.5381 -DE/DX =    0.0         !
! D37   D(25,11,12,13)   61.1993  -30.5072   78.8469 -DE/DX =    0.0         !
! D38   D(25,11,12,14)  -116.5798  148.0333  -99.2395 -DE/DX =    0.0         !
! D39   D(27,11,12,13)   -39.0105 -110.8288  -38.5656 -DE/DX =    0.0         !
! D40   D(27,11,12,14)   143.2104   67.7118  143.348  -DE/DX =    0.0         !
! D41   D(12,11,23,1)   -139.6723  179.1567 -122.118  -DE/DX =    0.0         !
! D42   D(12,11,23,24)   53.3793   -1.9154   80.8656 -DE/DX =    0.0         !
! D43   D(25,11,23,1)    -5.3201    0.3853   -9.6387 -DE/DX =    0.0         !
! D44   D(25,11,23,24)  -172.2685  179.3132 -166.655  -DE/DX =    0.0         !
! D45   D(27,11,23,1)    87.493    87.7433  100.4356 -DE/DX =    0.0         !
! D46   D(27,11,23,24)   -79.4554  -93.3289  -56.5808 -DE/DX =    0.0         !
! D47   D(12,11,25,2)    138.04   -179.3898  127.3725 -DE/DX =    0.0         !
! D48   D(12,11,25,26)     5.2825    2.7356    4.8925 -DE/DX =    0.0         !
! D49   D(23,11,25,2)      2.7537   -0.5974    7.9782 -DE/DX =    0.0         !
! D50   D(23,11,25,26)  -130.0038 -178.472  -114.5018 -DE/DX =    0.0         !
! D51   D(27,11,25,2)   -109.0155  -98.9018 -108.9771 -DE/DX =    0.0         !
! D52   D(27,11,25,26)   118.227    83.2237  128.5429 -DE/DX =    0.0         !
! D53   D(12,11,27,28)     4.7653 -118.0046   -1.9582 -DE/DX =    0.0         !
! D54   D(12,11,27,29)   116.2223   77.2428  113.4631 -DE/DX =    0.0         !
! D55   D(23,11,27,28)   142.4373    9.8264  135.6412 -DE/DX =    0.0         !
! D56   D(23,11,27,29)  -106.1056 -154.9262 -108.9374 -DE/DX =    0.0         !
! D57   D(25,11,27,28)  -115.9835  114.4362 -120.2837 -DE/DX =    0.0         !
! D58   D(25,11,27,29)    -4.5265  -50.3164   -4.8624 -DE/DX =    0.0         !
! D59   D(11,12,13,15)  -178.4628  178.9023 -178.5088 -DE/DX =    0.0         !
! D60   D(11,12,13,16)     0.7972   -1.7859    1.1352 -DE/DX =    0.0         !
! D61   D(14,12,13,15)    -0.6188    0.3172   -0.3359 -DE/DX =    0.0         !
! D62   D(14,12,13,16)   178.6412  179.6289  179.3081 -DE/DX =    0.0         !
! D63   D(11,12,14,17)   178.8036 -178.6489  178.7199 -DE/DX =    0.0         !
! D64   D(11,12,14,18)    -0.5655    0.4223   -1.3343 -DE/DX =    0.0         !
! D65   D(13,12,14,17)     0.9055   -0.0586    0.5553 -DE/DX =    0.0         !
! D66   D(13,12,14,18)  -178.4636  179.0126 -179.4989 -DE/DX =    0.0         !
! D67   D(12,13,15,19)    -0.0514   -0.3391   -0.0269 -DE/DX =    0.0         !
! D68   D(12,13,15,20)   179.9643  179.719   179.9375 -DE/DX =    0.0         !
! D69   D(16,13,15,19)  -179.3257 -179.6546 -179.675  -DE/DX =    0.0         !
! D70   D(16,13,15,20)     0.69      0.4034    0.2894 -DE/DX =    0.0         !
! D71   D(12,14,17,19)    -0.5238   -0.1772   -0.4129 -DE/DX =    0.0         !
! D72   D(12,14,17,21)   179.7193  179.7068  179.6951 -DE/DX =    0.0         !
! D73   D(18,14,17,19)   178.8399 -179.2521  179.6418 -DE/DX =    0.0         !
! D74   D(18,14,17,21)    -0.917     0.6319   -0.2501 -DE/DX =    0.0         !
! D75   D(13,15,19,17)     0.4607    0.0948    0.1864 -DE/DX =    0.0         !
! D76   D(13,15,19,22)  -179.771  -179.7822 -179.9873 -DE/DX =    0.0         !
! D77   D(20,15,19,17)  -179.555  -179.9633 -179.778  -DE/DX =    0.0         !
! D78   D(20,15,19,22)     0.2134    0.1596    0.0483 -DE/DX =    0.0         !
! D79   D(14,17,19,15)    -0.1802    0.1593    0.028  -DE/DX =    0.0         !
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 ! D80   D(14,17,19,22)  -179.9481 -179.9637 -179.7984 -DE/DX =    0.0         !
 ! D81   D(21,17,19,15)   179.5765 -179.7244  179.9201 -DE/DX =    0.0         !
 ! D82   D(21,17,19,22)    -0.1914    0.1526    0.0937 -DE/DX =    0.0         !
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GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradG
radGrad
%nprocshared=2
 Will use up to    2 processors via shared memory.
 %mem=1GB
 %chk=T:\CHM\deg013\Thusini\Reproducing data of li et. al paper\-BDAB-1st
reactio
 n7-20\TPH-01-46-FREQ-QST3-BDAB-W1.chk
 ----------------------------------------
 # freq wb97xd/6-31g(d,p) geom=connectivity
 ----------------------------------------
------------------
 - Thermochemistry -
 ------------------
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.
Zero-point correction=                          0.233780 (Hartree/Particle)
 Thermal correction to Energy=                  0.246430
 Thermal correction to Enthalpy=                0.247374
 Thermal correction to Gibbs Free Energy=       0.194075
 Sum of electronic and zero-point Energies=          -674.312544
 Sum of electronic and thermal Energies=             -674.299894
 Sum of electronic and thermal Enthalpies=           -674.298950
 Sum of electronic and thermal Free Energies=        -674.352249
```

IRC1-D

```
%nprocshared=3
 Will use up to    3 processors via shared memory.
 %mem=1GB
 %chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\TS1-
checking\TS1
 -D\IRC1- of TS1-D using TPH-01-46-FREQ-QST3-BDAB-W1.chk
 ----------------------------------------
 # irc=(maxpoints=15,calcfc) wb97xd/6-31g(d,p)
 ----------------------------------------
 1/10=4,14=-1,18=10,26=3,38=1,42=15,44=3/1,23;
 2/12=2,17=6,18=5,29=1,40=1/2;
 3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
 4//1;
 5/5=2,38=5/2;
```

8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1,13=1/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7/10=1,18=20,25=1/1,2,3,16;
1/10=4,14=-1,18=10,26=3,42=15,44=3/23(2);
2/29=1/2;
99/5=20/99;
2/29=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1,13=1/2;
7/10=1,18=20,25=1/1,2,3,16;
1/14=-1,18=10,26=3,42=15,44=3/23(-8);
2/29=1/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/5=20,9=1/99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	1.88354	0.5855	0.40661
C	1.89725	-0.55155	-0.42207
C	3.03307	-0.94493	-1.09868
C	4.20043	-0.18854	-0.94409
C	4.20157	0.92534	-0.11092
C	3.05138	1.32352	0.57432
H	3.01973	-1.82674	-1.73263
H	5.10466	-0.47822	-1.46811
H	5.11401	1.50077	0.01148
H	3.06311	2.19914	1.21604
B	-0.30139	-0.30727	0.57114
C	-1.81	-0.01001	0.15276
C	-2.75751	-1.02732	-0.0322
C	-2.22799	1.30371	-0.09134
C	-4.0627	-0.75102	-0.42828
H	-2.478	-2.06952	0.12272
C	-3.53176	1.59415	-0.48207
H	-1.50818	2.11023	0.01933
C	-4.45474	0.56609	-0.65007
H	-4.77398	-1.56036	-0.56389
H	-3.82726	2.6239	-0.65966

H	-5.47261	0.78788	-0.95557
N	0.6197	0.79691	0.92153
H	0.46641	1.51963	1.60259
N	0.61356	-1.18468	-0.39245
H	0.25177	-1.47392	-1.29353
O	-0.23261	-1.52506	1.66972
H	-1.08817	-1.92966	1.84742
H	0.32826	-1.90154	0.69297

IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC-IRC

TS2-D

%nprocshared=6
Will use up to 6 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thusini\Reproducing data of li et. al paper\BDAB-product form
ation\TPH-01-46Trial 02--OPT-QST3-BDAB-product formation-9-14--GAS PHASE-8-18.ch
k
---
opt=(calcall,qst3) wb97xd/6-31g(d,p) geom=connectivity

1/5=1,10=4,14=-1,18=20,26=3,27=203,38=1,57=2/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
4//1;
5/5=2,38=5/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;
10/6=1/2;
6/7=2,8=2,9=2,10=2,18=1,28=1/1;
7/10=1,25=1/1,2,3,16;
1/5=1,10=4,14=-1,18=20,26=3,27=203/3(3);
2/9=110/2;
7/8=1,9=1,25=1,44=-1/16;
99//99;
2/9=110/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=2,74=-58,140=1/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
8/6=4,10=90,11=11/1;
11/6=1,8=1,9=11,15=111,16=1/1,2,10;

```
10/6=1/2;
7/10=1,25=1/1,2,3,16;
1/5=1,10=4,14=-1,18=20,26=3,27=203/3(-8);
2/9=110/2;
6/7=2,8=2,9=2,10=2,18=1,19=2,28=1/1;
7/8=1,9=1,25=1,44=-1/16;
99//99;
```

Title Card Required

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-0.3875	0.55	0.
C	0.33773	1.75651	0.04158
C	1.73009	1.71237	-0.05689
C	2.41166	0.50694	-0.16252
C	1.70017	-0.68708	-0.16454
C	0.31379	-0.65408	-0.08685
H	2.28353	2.64772	-0.0329
H	3.49429	0.50475	-0.23249
H	2.21492	-1.63873	-0.23947
H	-0.25169	-1.58203	-0.11386
C	-4.32289	0.92481	-0.30557
C	-5.30087	1.34315	-1.21921
C	-4.75174	0.21712	0.82648
C	-6.64594	1.05003	-1.02293
H	-4.99294	1.90778	-2.09436
C	-6.09694	-0.07314	1.03605
H	-4.02726	-0.0997	1.5744
C	-7.04657	0.34017	0.10658
H	-7.38456	1.3779	-1.74794
H	-6.40434	-0.61624	1.9245
H	-8.09701	0.11641	0.26526
B	-2.81113	1.30272	-0.5523
O	-2.57197	2.39959	-1.3355
H	-1.65426	2.71866	-1.24579
O	-3.01643	3.6623	1.27709
H	-3.18027	3.64219	0.32473
H	-3.6391	3.01435	1.62047
N	-1.79796	0.51974	0.08072
N	-0.34112	2.98858	0.11507
H	-1.09487	3.02228	0.80518
H	0.28654	3.76829	0.25887
H	-2.13111	-0.34482	0.48271

Add virtual bond connecting atoms O23 and H26 Dist= 4.08D+00.

Add virtual bond connecting atoms H30 and O25 Dist= 3.93D+00.
Add virtual bond connecting atoms H30 and H26 Dist= 4.21D+00.

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.68013	0.07661	0.84292
C	-2.61925	-0.51441	-0.02915
C	-3.49254	1.6911	-0.54996
C	-3.51728	0.30621	-0.70751
C	-2.54828	2.27024	0.28759
C	-1.64933	1.46289	0.98136
H	-4.20117	2.30844	-1.09201
H	-4.24371	-0.15094	-1.37508
H	-2.50997	3.34731	0.41374
H	-0.91168	1.90912	1.64349
C	1.99449	-0.36775	-0.25555
C	1.4368	0.88913	-0.52793
C	3.35568	-0.41763	0.07189
C	2.20073	2.04929	-0.46133
H	0.37866	0.97331	-0.76344
C	4.13132	0.73677	0.13031
H	3.82935	-1.37809	0.26607
C	3.5521	1.97456	-0.13277
H	1.74062	3.01181	-0.6627
H	5.18658	0.67045	0.37691
H	4.15183	2.87832	-0.08454
B	1.12653	-1.68491	-0.32927
O	1.39712	-2.79131	0.42663
H	2.04233	-2.60273	1.10976
O	0.13598	-1.85149	-1.2682
H	0.02469	-1.07121	-1.81491
H	-0.35598	-0.33982	2.32351
N	-0.76239	-0.75538	1.49736
N	-2.63193	-1.92001	-0.12215
H	-3.37014	-2.25564	-0.72646
H	-1.73576	-2.27492	-0.45254
H	-1.14886	-1.67275	1.69139

Add virtual bond connecting atoms H31 and O25 Dist= 3.94D+00.

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-1.62832	0.21459	-0.49397
C	-2.72722	-0.58132	-0.14976
C	-3.94362	0.01489	0.15808
C	-4.06578	1.40322	0.13586
C	-2.97373	2.19407	-0.19895
C	-1.75602	1.59494	-0.5155
H	-4.79591	-0.60627	0.4236
H	-5.01946	1.85931	0.37894
H	-3.0664	3.27444	-0.2203
H	-0.88706	2.18305	-0.79164
C	2.0234	-0.19592	0.15898
C	2.20771	1.1595	0.46448
C	3.12565	-0.91259	-0.31719
C	3.44317	1.77787	0.30322
H	1.36551	1.74677	0.82789
C	4.36698	-0.30285	-0.48033
H	3.00435	-1.96359	-0.56338
C	4.52832	1.04423	-0.17029
H	3.56191	2.8308	0.54132
H	5.20992	-0.87854	-0.85109
H	5.49475	1.52216	-0.29893
B	0.60477	-0.86608	0.37947
O	-0.01914	-0.80744	1.62748
H	0.46692	-0.25038	2.23602
O	0.44993	-2.27935	-0.23335
H	-0.07646	-2.801	0.38506
H	-0.30838	-1.59333	-0.86333
N	-0.34375	-0.41071	-0.84007
N	-2.50964	-2.03512	-0.14775
H	-3.13234	-2.46627	-0.80071
H	-2.68404	-2.39701	0.76802
H	0.36115	-0.09885	-0.203

GradGradGradG

-- Stationary point found.

Optimized Parameters (Angstroms and Degrees)				
Name	Definition	TS	Reactant	Product
R1	R(1,2)	1.4079	1.4083	1.4113
R2	R(1,6)	1.3938	1.3961	1.3935
R3	R(1,28)	1.4236	1.4131	1.401
R4	R(2,3)	1.3956	1.3965	2.4286
R5	R(2,4)	2.4325	2.4299	1.3929
R6	R(2,29)	1.4147	1.4086	1.4087
R7	R(3,4)	1.3904	1.3888	1.394
R8	R(3,5)	2.4017	2.402	1.3887
R9	R(3,7)	1.0872	1.0871	1.0849
R10	R(4,5)	1.3887	1.3899	2.4055
R11	R(4,8)	1.0849	1.0849	1.0873
R12	R(5,6)	1.3904	1.389	1.3933
R13	R(5,9)	1.0847	1.0845	1.0851
R14	R(6,10)	1.0873	1.087	1.087
R15	R(11,12)	1.403	1.4022	1.4018
R16	R(11,13)	1.399	1.4022	1.4009
R17	R(11,22)	1.5962	1.5777	1.5791
R18	R(12,14)	1.3914	1.3906	1.3907
R19	R(12,15)	1.0887	1.0861	1.0873
R20	R(13,16)	1.3929	1.392	1.392
R21	R(13,17)	1.086	1.0884	1.0884
R22	R(14,18)	1.3929	1.3929	1.3927
R23	R(14,19)	1.0861	1.0857	1.0857
R24	R(16,18)	1.3918	1.3916	1.3917
R25	R(16,20)	1.0862	1.0857	1.0857
R26	R(18,21)	1.0858	1.0857	1.0857
R27	R(22,23)	1.4207	1.3688	1.367
R28	R(22,25)	1.6149	2.9927	1.375
R29	R(22,28)	1.6046	1.4284	2.7872
R30	R(23,24)	0.9574	0.9757	0.9584
R31	R(23,26)	2.4915	2.1611	3.1411
R32	R(25,26)	0.9664	0.9666	0.9592
R33	R(25,27)	1.1877	0.962	3.9278
R34	R(25,30)	3.8987	2.0796	3.5707
R35	R(25,31)	2.8407	3.458	2.0852
R36	R(26,30)	3.1944	2.228	3.7566
R37	R(27,28)	1.3374	3.4617	1.0101
R38	R(28,32)	1.0142	1.01	1.0142
R39	R(29,30)	1.0123	1.0225	1.0113

Derivative Info. -DE/DX = 0.0 for all rows

```
! R40   R(29,31)         1.0198    1.0112    1.0189 -DE/DX =    0.0         !
! A1    A(2,1,6)        119.275   118.8175  119.518  -DE/DX =    0.0         !
! A2    A(2,1,28)       121.1222  122.0503  118.4156 -DE/DX =    0.0         !
! A3    A(6,1,28)       119.5024  119.1084  121.998  -DE/DX =    0.0         !
! A4    A(1,2,3)        118.606   118.9643   89.5124 -DE/DX =    0.0         !
! A5    A(1,2,4)         89.4864   89.7987  118.8982 -DE/DX =    0.0         !
! A6    A(1,2,29)       119.7883  120.1781  117.6864 -DE/DX =    0.0         !
! A7    A(3,2,29)       121.5785  120.7843  152.7129 -DE/DX =    0.0         !
! A8    A(4,2,29)       150.6839  149.9407  123.3594 -DE/DX =    0.0         !
! A9    A(2,3,4)        121.6399  121.4729   29.3602 -DE/DX =    0.0         !
! A10   A(2,3,7)        118.5906  118.609   149.1762 -DE/DX =    0.0         !
! A11   A(4,3,5)         30.1886   30.1944  119.6382 -DE/DX =    0.0         !
! A12   A(4,3,7)        119.7694  119.9104  119.8162 -DE/DX =    0.0         !
! A13   A(5,3,7)        149.9466  150.0911  120.5404 -DE/DX =    0.0         !
! A14   A(2,4,3)         29.2397   29.3527  121.2521 -DE/DX =    0.0         !
! A15   A(2,4,8)        149.0268  149.1142  118.8193 -DE/DX =    0.0         !
! A16   A(3,4,5)        119.5821  119.6383   30.117  -DE/DX =    0.0         !
! A17   A(3,4,8)        119.7878  119.7622  119.9275 -DE/DX =    0.0         !
! A18   A(5,4,8)        120.6253  120.5966  150.0365 -DE/DX =    0.0         !
! A19   A(3,5,6)         89.1862   89.2087  119.8265 -DE/DX =    0.0         !
! A20   A(3,5,9)        150.9616  150.8925  120.5346 -DE/DX =    0.0         !
! A21   A(4,5,6)        119.4103  119.37    89.5866 -DE/DX =    0.0         !
! A22   A(4,5,9)        120.7383  120.7266  150.7768 -DE/DX =    0.0         !
! A23   A(6,5,9)        119.8507  119.8982  119.6366 -DE/DX =    0.0         !
! A24   A(1,6,5)        121.4474  121.6922  120.8448 -DE/DX =    0.0         !
! A25   A(1,6,10)        118.7753  118.4556  118.9391 -DE/DX =    0.0         !
! A26   A(5,6,10)        119.7683  119.8403  120.2159 -DE/DX =    0.0         !
! A27   A(12,11,13)      117.6874  117.5993  117.6395 -DE/DX =    0.0         !
! A28   A(12,11,22)      119.1205  119.6665  121.3413 -DE/DX =    0.0         !
! A29   A(13,11,22)      123.1873  122.6971  121.0159 -DE/DX =    0.0         !
! A30   A(11,12,14)      121.4902  121.3175  121.3431 -DE/DX =    0.0         !
! A31   A(11,12,15)      119.2499  118.8421  119.9134 -DE/DX =    0.0         !
! A32   A(14,12,15)      119.2599  119.8404  118.7095 -DE/DX =    0.0         !
! A33   A(11,13,16)      121.2294  121.4888  121.4464 -DE/DX =    0.0         !
! A34   A(11,13,17)      118.9102  119.874   119.7351 -DE/DX =    0.0         !
! A35   A(16,13,17)      119.8604  118.6258  118.8063 -DE/DX =    0.0         !
! A36   A(12,14,18)      119.8012  120.0063  119.9689 -DE/DX =    0.0         !
! A37   A(12,14,19)      120.1344  120.0102  119.8626 -DE/DX =    0.0         !
! A38   A(18,14,19)      120.0643  119.983   120.1682 -DE/DX =    0.0         !
! A39   A(13,16,18)      120.1087  119.7986  119.8511 -DE/DX =    0.0         !
! A40   A(13,16,20)      119.9917  120.0735  120.03   -DE/DX =    0.0         !
! A41   A(18,16,20)      119.8996  120.1272  120.1184 -DE/DX =    0.0         !
! A42   A(14,18,16)      119.6831  119.7823  119.7458 -DE/DX =    0.0         !
! A43   A(14,18,21)      120.1212  120.1221  120.1182 -DE/DX =    0.0         !
! A44   A(16,18,21)      120.1957  120.094   120.1358 -DE/DX =    0.0         !
! A45   A(11,22,23)      117.3531  116.6687  122.7155 -DE/DX =    0.0         !
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! A46   A(11,22,25)     109.9593   91.5772  121.9316 -DE/DX =    0.0         !
! A47   A(11,22,28)     112.3492  118.6243   93.6542 -DE/DX =    0.0         !
! A48   A(23,22,25)     111.5677   74.3324  114.9701 -DE/DX =    0.0         !
! A49   A(23,22,28)     112.7434  124.6725   92.3887 -DE/DX =    0.0         !
! A50   A(22,23,24)     110.7185  111.9475  111.6013 -DE/DX =    0.0         !
! A51   A(22,23,26)      58.4947   88.3963   22.4394 -DE/DX =    0.0         !
! A52   A(24,23,26)     124.0187   90.3491  134.0305 -DE/DX =    0.0         !
! A53   A(22,25,26)     108.388    52.6216  111.9773 -DE/DX =    0.0         !
! A54   A(22,25,31)      66.2251   77.2115  113.8385 -DE/DX =    0.0         !
! A55   A(26,25,27)     103.9327  103.1773  101.162  -DE/DX =    0.0         !
! A56   A(26,25,31)      45.8075   82.6704  106.4978 -DE/DX =    0.0         !
! A57   A(27,25,30)      68.3775  118.1497   77.3988 -DE/DX =    0.0         !
! A58   A(23,26,25)      80.0987  136.153    25.4636 -DE/DX =    0.0         !
! A59   A(23,26,30)      77.0682   75.0618   90.8839 -DE/DX =    0.0         !
! A60   A(1,28,22)      126.8829  132.1393  109.6246 -DE/DX =    0.0         !
! A61   A(1,28,27)      120.918   122.7408  113.6592 -DE/DX =    0.0         !
! A62   A(1,28,32)      110.1023  111.7348  112.1426 -DE/DX =    0.0         !
! A63   A(22,28,32)     110.4903  114.3086   94.7016 -DE/DX =    0.0         !
! A64   A(27,28,32)     113.1607  105.3314  111.6516 -DE/DX =    0.0         !
! A65   A(2,29,30)      110.9522  114.7893  112.1571 -DE/DX =    0.0         !
! A66   A(2,29,31)      109.3955  112.5008  111.1627 -DE/DX =    0.0         !
! A67   A(30,29,31)     109.4801  109.6434  109.4297 -DE/DX =    0.0         !
! A68   A(25,30,29)      28.7256  147.611    48.4214 -DE/DX =    0.0         !
! A69   A(26,30,29)      38.9921  123.6143   53.7624 -DE/DX =    0.0         !
! A70   A(25,31,29)      91.9138   54.9262  147.7356 -DE/DX =    0.0         !
! D1    D(6,1,2,3)        1.9772    2.4247   -1.2163 -DE/DX =    0.0         !
! D2    D(6,1,2,4)        1.7459    1.6741   -1.5579 -DE/DX =    0.0         !
! D3    D(6,1,2,29)    -179.8903  179.3356 -178.929  -DE/DX =    0.0         !
! D4    D(28,1,2,3)    -174.362  -179.3639 -178.2677 -DE/DX =    0.0         !
! D5    D(28,1,2,4)    -174.5933  179.8854 -178.6093 -DE/DX =    0.0         !
! D6    D(28,1,2,29)      3.7705   -2.453    4.0196 -DE/DX =    0.0         !
! D7    D(2,1,6,5)       -1.9556   -1.5389    1.1013 -DE/DX =    0.0         !
! D8    D(2,1,6,10)     179.1327  179.7172 -179.0332 -DE/DX =    0.0         !
! D9    D(28,1,6,5)     174.4437 -179.8038  178.0433 -DE/DX =    0.0         !
! D10   D(28,1,6,10)     -4.468     1.4523   -2.0912 -DE/DX =    0.0         !
! D11   D(2,1,28,22)     -54.8014   44.6275   72.1835 -DE/DX =    0.0         !
! D12   D(2,1,28,27)      32.3883  -25.4748 -159.4662 -DE/DX =    0.0         !
! D13   D(2,1,28,32)     167.4117 -151.9683  -31.6467 -DE/DX =    0.0         !
! D14   D(6,1,28,22)     128.8676 -137.1661 -104.7908 -DE/DX =    0.0         !
! D15   D(6,1,28,27)    -143.9427  152.7315   23.5594 -DE/DX =    0.0         !
! D16   D(6,1,28,32)      -8.9193   26.238   151.3789 -DE/DX =    0.0         !
! D17   D(1,2,3,4)        -0.4752   -1.5401 -179.3906 -DE/DX =    0.0         !
! D18   D(1,2,3,7)       179.6378  179.4723 -179.6871 -DE/DX =    0.0         !
! D19   D(29,2,3,4)     -178.5728 -178.4317   -3.8118 -DE/DX =    0.0         !
! D20   D(29,2,3,7)        1.5403    2.5807   -4.1083 -DE/DX =    0.0         !
! D21   D(1,2,4,3)       179.5828  178.6526    0.6961 -DE/DX =    0.0         !
```

```
! D22   D(1,2,4,8)       179.0439  179.1693 -179.6821 -DE/DX =    0.0         !
! D23   D(29,2,4,3)       2.4837    2.6906  177.9089 -DE/DX =    0.0         !
! D24   D(29,2,4,8)       1.9448    3.2073   -2.4693 -DE/DX =    0.0         !
! D25   D(1,2,29,30)    -173.9934   46.2989  176.6372 -DE/DX =    0.0         !
! D26   D(1,2,29,31)      65.117   172.6052  -60.4888 -DE/DX =    0.0         !
! D27   D(3,2,29,30)      4.0821 -136.8472    1.6312 -DE/DX =    0.0         !
! D28   D(3,2,29,31)    -116.8075  -10.5409  124.5052 -DE/DX =    0.0         !
! D29   D(4,2,29,30)      2.6636 -138.3735   -0.6072 -DE/DX =    0.0         !
! D30   D(4,2,29,31)    -118.226   -12.0672  122.2668 -DE/DX =    0.0         !
! D31   D(2,3,4,5)       -1.1107   -0.315    -0.6498 -DE/DX =    0.0         !
! D32   D(2,3,4,8)      179.6804 -179.6945 -179.6177 -DE/DX =    0.0         !
! D33   D(5,3,4,2)        1.1107    0.315     0.6498 -DE/DX =    0.0         !
! D34   D(5,3,4,8)     -179.2088 -179.3795 -178.9679 -DE/DX =    0.0         !
! D35   D(7,3,4,2)      179.8856  178.9747  179.8249 -DE/DX =    0.0         !
! D36   D(7,3,4,5)      178.7749  178.6597  179.175  -DE/DX =    0.0         !
! D37   D(7,3,4,8)       -0.4339   -0.7198    0.2072 -DE/DX =    0.0         !
! D38   D(4,3,5,6)     -178.9858 -178.9149   -1.1265 -DE/DX =    0.0         !
! D39   D(4,3,5,9)        1.5595    0.7284  179.4286 -DE/DX =    0.0         !
! D40   D(7,3,5,6)      178.8905  178.7547  179.7046 -DE/DX =    0.0         !
! D41   D(7,3,5,9)       -0.5642   -1.602     0.2597 -DE/DX =    0.0         !
! D42   D(3,4,5,6)        1.1642    1.2451  179.0227 -DE/DX =    0.0         !
! D43   D(3,4,5,9)     -179.1194 -179.5878   -1.0081 -DE/DX =    0.0         !
! D44   D(8,4,5,6)     -179.6337 -179.3807 -179.1861 -DE/DX =    0.0         !
! D45   D(8,4,5,9)        0.0827   -0.2136    0.7831 -DE/DX =    0.0         !
! D46   D(3,5,6,1)        0.954     0.3144    0.2515 -DE/DX =    0.0         !
! D47   D(3,5,6,10)     179.8551  179.0413 -179.6122 -DE/DX =    0.0         !
! D48   D(4,5,6,1)        0.3679   -0.3113   -0.3159 -DE/DX =    0.0         !
! D49   D(4,5,6,10)     179.2689  178.4156  179.8204 -DE/DX =    0.0         !
! D50   D(9,5,6,1)     -179.3511 -179.4854  179.7015 -DE/DX =    0.0         !
! D51   D(9,5,6,10)      -0.4501   -0.7586   -0.1623 -DE/DX =    0.0         !
! D52   D(13,11,12,14)   -0.0438   -0.9862   -0.7308 -DE/DX =    0.0         !
! D53   D(13,11,12,15)  179.8848  178.9507 -178.582  -DE/DX =    0.0         !
! D54   D(22,11,12,14)  179.1847 -178.8296  179.9157 -DE/DX =    0.0         !
! D55   D(22,11,12,15)   -0.8868    1.1073    2.0645 -DE/DX =    0.0         !
! D56   D(12,11,13,16)    0.1035    0.5465    0.1897 -DE/DX =    0.0         !
! D57   D(12,11,13,17) -179.8303 -178.2024 -178.5217 -DE/DX =    0.0         !
! D58   D(22,11,13,16) -179.0911  178.3196  179.5454 -DE/DX =    0.0         !
! D59   D(22,11,13,17)    0.975    -0.4292    0.834  -DE/DX =    0.0         !
! D60   D(12,11,22,23)  -60.8909   23.4848 -151.3775 -DE/DX =    0.0         !
! D61   D(12,11,22,25)  170.1921   96.7172   36.0849 -DE/DX =    0.0         !
! D62   D(12,11,22,28)   72.2118 -158.5511  -56.1758 -DE/DX =    0.0         !
! D63   D(13,11,22,23)  118.2927 -154.2441   29.2907 -DE/DX =    0.0         !
! D64   D(13,11,22,25)  -10.6243  -81.0117 -143.2468 -DE/DX =    0.0         !
! D65   D(13,11,22,28) -108.6046   23.72    124.4924 -DE/DX =    0.0         !
! D66   D(11,12,14,18)   -0.0091    0.7175    0.7095 -DE/DX =    0.0         !
! D67   D(11,12,14,19)  179.9032 -179.5331 -179.0933 -DE/DX =    0.0         !
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! D68   D(15,12,14,18)  -179.9376 -179.2187  178.5859 -DE/DX =    0.0         !
! D69   D(15,12,14,19)    -0.0254    0.5307   -1.2169 -DE/DX =    0.0         !
! D70   D(11,13,16,18)    -0.1108    0.162     0.3711 -DE/DX =    0.0         !
! D71   D(11,13,16,20)   179.8903 -179.5465 -179.3954 -DE/DX =    0.0         !
! D72   D(17,13,16,18)   179.8225  178.926   179.0942 -DE/DX =    0.0         !
! D73   D(17,13,16,20)    -0.1764   -0.7825   -0.6724 -DE/DX =    0.0         !
! D74   D(12,14,18,16)     0.0041    0.0217   -0.1277 -DE/DX =    0.0         !
! D75   D(12,14,18,21)   179.9221  179.5653  179.7193 -DE/DX =    0.0         !
! D76   D(19,14,18,16)  -179.9082 -179.7277  179.6745 -DE/DX =    0.0         !
! D77   D(19,14,18,21)     0.0098   -0.1842   -0.4785 -DE/DX =    0.0         !
! D78   D(13,16,18,14)     0.0548   -0.4538   -0.4031 -DE/DX =    0.0         !
! D79   D(13,16,18,21)  -179.8631 -179.9974  179.7499 -DE/DX =    0.0         !
! D80   D(20,16,18,14)  -179.9463  179.2545  179.3632 -DE/DX =    0.0         !
! D81   D(20,16,18,21)     0.1358   -0.2891   -0.4838 -DE/DX =    0.0         !
! D82   D(11,22,23,24)   -16.4725  164.1733   11.564  -DE/DX =    0.0         !
! D83   D(11,22,23,26)  -134.4893   74.4431 -169.9809 -DE/DX =    0.0         !
! D84   D(25,22,23,24)   111.6788   80.4242 -175.4198 -DE/DX =    0.0         !
! D85   D(28,22,23,24)  -149.3998  -13.6537  -84.3256 -DE/DX =    0.0         !
! D86   D(28,22,23,26)    92.5835 -103.3838   94.1295 -DE/DX =    0.0         !
! D87   D(11,22,25,26)   146.8209  -90.2442   -2.8303 -DE/DX =    0.0         !
! D88   D(11,22,25,31)   165.1731  179.2529 -123.7016 -DE/DX =    0.0         !
! D89   D(23,22,25,26)    14.8164   27.0528 -175.907  -DE/DX =    0.0         !
! D90   D(23,22,25,31)    33.1685  -63.45     63.2217 -DE/DX =    0.0         !
! D91   D(11,22,28,1)   -134.2377  175.715    81.7503 -DE/DX =    0.0         !
! D92   D(11,22,28,32)     3.4188   12.6403 -162.7293 -DE/DX =    0.0         !
! D93   D(23,22,28,1)      1.0804   -6.4972 -155.2453 -DE/DX =    0.0         !
! D94   D(23,22,28,32)   138.7369 -169.5719  -39.7248 -DE/DX =    0.0         !
! D95   D(22,23,26,25)    10.0299   44.0998 -170.7908 -DE/DX =    0.0         !
! D96   D(22,23,26,30)  -126.4655   78.6535 -131.076  -DE/DX =    0.0         !
! D97   D(24,23,26,25)   -84.9556  -67.8466 -168.7928 -DE/DX =    0.0         !
! D98   D(24,23,26,30)   138.549   -33.293  -129.078  -DE/DX =    0.0         !
! D99   D(27,25,26,23)   -84.2935  -81.8796   59.7823 -DE/DX =    0.0         !
! D100  D(26,25,27,30)    13.9542   92.2821   91.3394 -DE/DX =    0.0         !
! D101  D(27,25,30,29)   -42.3283  129.0358   -4.7761 -DE/DX =    0.0         !
! D102  D(22,25,31,29)   121.1898  -12.4085   93.3159 -DE/DX =    0.0         !
! D103  D(26,25,31,29)   -83.4372  -65.6495  -30.5725 -DE/DX =    0.0         !
! D104  D(23,26,30,29)    49.0515   41.5447   46.5642 -DE/DX =    0.0         !
! D105  D(2,29,30,25)    159.3354 -139.9524  101.5347 -DE/DX =    0.0         !
! D106  D(2,29,30,26)    165.1696 -126.6283   83.802  -DE/DX =    0.0         !
! D107  D(31,29,30,25)   -79.825    92.2819  -22.3128 -DE/DX =    0.0         !
! D108  D(31,29,30,26)   -73.9908  105.6061  -40.0455 -DE/DX =    0.0         !
! D109  D(2,29,31,25)    -98.7321 -152.1905  -10.0778 -DE/DX =    0.0         !
! D110  D(30,29,31,25)   139.4879  -23.1604  114.3522 -DE/DX =    0.0         !
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GradGradGradG

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1
O 0. 0. 0.11785
H 0. 0.75761 -0.47138
H 0. -0.75761 -0.47138

GradGradGradG

-- Stationary point found.

! Optimized Parameters !
! (Angstroms and Degrees) !

Name	Definition	TS	Reactant	Product	Derivative Info.
R1	R(1,2)	1.4079	1.4105	1.4052	-DE/DX = 0.0
R2	R(1,6)	1.3938	1.3977	1.3845	-DE/DX = 0.0
R3	R(1,28)	1.4236	1.4052	1.4342	-DE/DX = 0.0
R4	R(2,3)	1.3956	1.3957	1.3971	-DE/DX = 0.0
R5	R(2,29)	1.4147	1.424	1.4034	-DE/DX = 0.0
R6	R(3,4)	1.3904	1.3913	1.3889	-DE/DX = 0.0
R7	R(3,7)	1.0872	1.0878	1.0866	-DE/DX = 0.0
R8	R(4,5)	1.3887	1.389	1.3891	-DE/DX = 0.0
R9	R(4,8)	1.0849	1.0849	1.085	-DE/DX = 0.0
R10	R(5,6)	1.3904	1.3876	1.388	-DE/DX = 0.0
R11	R(5,9)	1.0847	1.0851	1.084	-DE/DX = 0.0
R12	R(6,10)	1.0873	1.0874	1.087	-DE/DX = 0.0
R13	R(11,12)	1.403	1.4038	1.4044	-DE/DX = 0.0
R14	R(11,13)	1.399	1.4	1.3995	-DE/DX = 0.0
R15	R(11,22)	1.5962	1.6008	1.6129	-DE/DX = 0.0
R16	R(12,14)	1.3914	1.3908	1.3936	-DE/DX = 0.0
R17	R(12,15)	1.0887	1.0885	1.0896	-DE/DX = 0.0
R18	R(13,16)	1.3929	1.3941	1.392	-DE/DX = 0.0
R19	R(13,17)	1.086	1.0862	1.086	-DE/DX = 0.0
R20	R(14,18)	1.3929	1.3924	1.3928	-DE/DX = 0.0
R21	R(14,19)	1.0861	1.086	1.0864	-DE/DX = 0.0
R22	R(16,18)	1.3918	1.3917	1.3923	-DE/DX = 0.0
R23	R(16,20)	1.0862	1.0862	1.0864	-DE/DX = 0.0
R24	R(18,21)	1.0858	1.0858	1.086	-DE/DX = 0.0
R25	R(22,23)	1.4207	1.4201	1.442	-DE/DX = 0.0
R26	R(22,25)	1.6149	1.7602	1.4822	-DE/DX = 0.0
R27	R(22,28)	1.6046	1.5131	1.6845	-DE/DX = 0.0
R28	R(23,24)	0.9574	0.9577	0.9572	-DE/DX = 0.0
R29	R(25,26)	0.9664	0.9708	0.9598	-DE/DX = 0.0
R30	R(25,27)	1.1877	0.981	1.8313	-DE/DX = 0.0
R31	R(27,28)	1.3374	1.9177	1.0234	-DE/DX = 0.0
R32	R(28,32)	1.0142	1.0113	1.0173	-DE/DX = 0.0
R33	R(29,30)	1.0123	1.0132	1.0113	-DE/DX = 0.0
R34	R(29,31)	1.0198	1.0197	1.0219	-DE/DX = 0.0
A1	A(2,1,6)	119.2749	118.5313	120.9941	-DE/DX = 0.0
A2	A(2,1,28)	121.1225	122.7003	120.5324	-DE/DX = 0.0
A3	A(6,1,28)	119.5022	118.7269	118.2982	-DE/DX = 0.0
A4	A(1,2,3)	118.606	118.9162	117.3698	-DE/DX = 0.0
A5	A(1,2,29)	119.7885	119.6725	120.8123	-DE/DX = 0.0

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! A6    A(3,2,29)      121.5783  121.4001  121.783  -DE/DX =    0.0         !
! A7    A(2,3,4)       121.6399  121.8026  121.6505 -DE/DX =    0.0         !
! A8    A(2,3,7)       118.5906  118.5749  118.4969 -DE/DX =    0.0         !
! A9    A(4,3,7)       119.7694  119.6225  119.8511 -DE/DX =    0.0         !
! A10   A(3,4,5)        119.582   119.2793  120.0425 -DE/DX =    0.0         !
! A11   A(3,4,8)        119.7878  119.9432  119.5896 -DE/DX =    0.0         !
! A12   A(5,4,8)        120.6254  120.7741  120.3624 -DE/DX =    0.0         !
! A13   A(4,5,6)        119.4104  119.5178  119.1748 -DE/DX =    0.0         !
! A14   A(4,5,9)        120.7383  120.6947  120.8567 -DE/DX =    0.0         !
! A15   A(6,5,9)        119.8508  119.7872  119.966  -DE/DX =    0.0         !
! A16   A(1,6,5)        121.4475  121.9402  120.7311 -DE/DX =    0.0         !
! A17   A(1,6,10)       118.7753  118.3293  119.2051 -DE/DX =    0.0         !
! A18   A(5,6,10)       119.7683  119.7304  120.0507 -DE/DX =    0.0         !
! A19   A(12,11,13)     117.6873  117.4221  117.4577 -DE/DX =    0.0         !
! A20   A(12,11,22)     119.1205  116.4916  122.855  -DE/DX =    0.0         !
! A21   A(13,11,22)     123.1873  126.0839  119.6556 -DE/DX =    0.0         !
! A22   A(11,12,14)     121.4902  121.7212  121.5379 -DE/DX =    0.0         !
! A23   A(11,12,15)     119.2499  119.1151  119.3567 -DE/DX =    0.0         !
! A24   A(14,12,15)     119.2599  119.1602  119.1048 -DE/DX =    0.0         !
! A25   A(11,13,16)     121.2294  121.2705  121.4724 -DE/DX =    0.0         !
! A26   A(11,13,17)     118.9102  119.2977  118.1693 -DE/DX =    0.0         !
! A27   A(16,13,17)     119.8603  119.4306  120.3582 -DE/DX =    0.0         !
! A28   A(12,14,18)     119.8012  119.7982  119.796  -DE/DX =    0.0         !
! A29   A(12,14,19)     120.1344  120.0843  120.1776 -DE/DX =    0.0         !
! A30   A(18,14,19)     120.0643  120.1168  120.0264 -DE/DX =    0.0         !
! A31   A(13,16,18)     120.1087  120.1984  120.0706 -DE/DX =    0.0         !
! A32   A(13,16,20)     119.9917  119.9195  120.0667 -DE/DX =    0.0         !
! A33   A(18,16,20)     119.8996  119.8821  119.8627 -DE/DX =    0.0         !
! A34   A(14,18,16)     119.683   119.5866  119.6651 -DE/DX =    0.0         !
! A35   A(14,18,21)     120.1212  120.1808  120.1207 -DE/DX =    0.0         !
! A36   A(16,18,21)     120.1957  120.2325  120.2141 -DE/DX =    0.0         !
! A37   A(11,22,23)     117.353   116.5135  114.9635 -DE/DX =    0.0         !
! A38   A(11,22,25)     109.9589  106.3067  112.9669 -DE/DX =    0.0         !
! A39   A(11,22,28)     112.3488  114.6464  108.61   -DE/DX =    0.0         !
! A40   A(23,22,25)     111.5686  105.7296  115.8612 -DE/DX =    0.0         !
! A41   A(23,22,28)     112.7434  116.1216  108.6079 -DE/DX =    0.0         !
! A42   A(25,22,28)      89.4782   93.8006   93.3275 -DE/DX =    0.0         !
! A43   A(22,23,24)     110.7184  110.5711  110.2271 -DE/DX =    0.0         !
! A44   A(22,25,26)     108.3877  103.717   109.5129 -DE/DX =    0.0         !
! A45   A(22,25,27)      72.9726   88.7663   72.224  -DE/DX =    0.0         !
! A46   A(26,25,27)     103.931   102.0129  104.0684 -DE/DX =    0.0         !
! A47   A(25,27,28)     127.5494  107.0109  104.2626 -DE/DX =    0.0         !
! A48   A(1,28,22)      126.8833  127.5837  127.0499 -DE/DX =    0.0         !
! A49   A(1,28,27)      120.9166  120.1788  109.2333 -DE/DX =    0.0         !
! A50   A(1,28,32)      110.1024  110.1257  110.4084 -DE/DX =    0.0         !
! A51   A(22,28,27)      69.9996   70.0449   90.1402 -DE/DX =    0.0         !
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! A52   A(22,28,32)     110.4905  111.2186  109.6978 -DE/DX =    0.0         !
! A53   A(27,28,32)     113.1615  112.1686  107.1026 -DE/DX =    0.0         !
! A54   A(2,29,30)      110.9521  110.307   111.5728 -DE/DX =    0.0         !
! A55   A(2,29,31)      109.3955  108.6563  110.2739 -DE/DX =    0.0         !
! A56   A(30,29,31)     109.4802  108.7497  110.8135 -DE/DX =    0.0         !
! D1    D(6,1,2,3)       1.9772    0.8368    1.9777 -DE/DX =    0.0         !
! D2    D(6,1,2,29)   -179.8901  179.6366  179.867  -DE/DX =    0.0         !
! D3    D(28,1,2,3)   -174.3618 -176.7889 -173.1286 -DE/DX =    0.0         !
! D4    D(28,1,2,29)     3.7709    2.0109    4.7608 -DE/DX =    0.0         !
! D5    D(2,1,6,5)      -1.9556   -1.1158   -1.6858 -DE/DX =    0.0         !
! D6    D(2,1,6,10)    179.1327  179.023   179.6261 -DE/DX =    0.0         !
! D7    D(28,1,6,5)    174.4435  176.6059  173.5272 -DE/DX =    0.0         !
! D8    D(28,1,6,10)    -4.4682   -3.2553   -5.1609 -DE/DX =    0.0         !
! D9    D(2,1,28,22)    -54.798   -51.7467  -51.4821 -DE/DX =    0.0         !
! D10   D(2,1,28,27)     32.3907   35.3517   53.9818 -DE/DX =    0.0         !
! D11   D(2,1,28,32)    167.414   168.038   171.5069 -DE/DX =    0.0         !
! D12   D(6,1,28,22)    128.8712  130.632   133.282  -DE/DX =    0.0         !
! D13   D(6,1,28,27)   -143.9401 -142.2696 -121.2541 -DE/DX =    0.0         !
! D14   D(6,1,28,32)     -8.9169   -9.5833   -3.729  -DE/DX =    0.0         !
! D15   D(1,2,3,4)       -0.4753    0.1592   -0.634  -DE/DX =    0.0         !
! D16   D(1,2,3,7)      179.6378 -179.8523  179.8188 -DE/DX =    0.0         !
! D17   D(29,2,3,4)    -178.573  -178.6191 -178.5015 -DE/DX =    0.0         !
! D18   D(29,2,3,7)       1.5401    1.3694    1.9513 -DE/DX =    0.0         !
! D19   D(1,2,29,30)   -173.9933 -173.2973 -175.4082 -DE/DX =    0.0         !
! D20   D(1,2,29,31)     65.1172   67.5798   60.9928 -DE/DX =    0.0         !
! D21   D(3,2,29,30)      4.0823    5.4719    2.3867 -DE/DX =    0.0         !
! D22   D(3,2,29,31)   -116.8072 -113.651  -121.2123 -DE/DX =    0.0         !
! D23   D(2,3,4,5)       -1.1107   -0.9128   -1.0218 -DE/DX =    0.0         !
! D24   D(2,3,4,8)      179.6806  179.7506  179.8286 -DE/DX =    0.0         !
! D25   D(7,3,4,5)      178.7749  179.0988  178.5194 -DE/DX =    0.0         !
! D26   D(7,3,4,8)       -0.4338   -0.2378   -0.6302 -DE/DX =    0.0         !
! D27   D(3,4,5,6)        1.1642    0.6441    1.3523 -DE/DX =    0.0         !
! D28   D(3,4,5,9)     -179.1192 -179.1759 -179.2272 -DE/DX =    0.0         !
! D29   D(8,4,5,6)     -179.6338  179.975  -179.5047 -DE/DX =    0.0         !
! D30   D(8,4,5,9)        0.0828    0.1551   -0.0842 -DE/DX =    0.0         !
! D31   D(4,5,6,1)        0.3678    0.3717   -0.018  -DE/DX =    0.0         !
! D32   D(4,5,6,10)     179.2689 -179.7691  178.659  -DE/DX =    0.0         !
! D33   D(9,5,6,1)     -179.3513 -179.8067 -179.4438 -DE/DX =    0.0         !
! D34   D(9,5,6,10)      -0.4502    0.0525   -0.7667 -DE/DX =    0.0         !
! D35   D(13,11,12,14)   -0.0437    0.553     0.0667 -DE/DX =    0.0         !
! D36   D(13,11,12,15)   179.8849  179.8604 -179.6372 -DE/DX =    0.0         !
! D37   D(22,11,12,14)   179.1854 -178.9242  178.0126 -DE/DX =    0.0         !
! D38   D(22,11,12,15)   -0.8861    0.3831   -1.6913 -DE/DX =    0.0         !
! D39   D(12,11,13,16)    0.1034   -0.5803    0.0383 -DE/DX =    0.0         !
! D40   D(12,11,13,17)  -179.8307  179.822   179.9328 -DE/DX =    0.0         !
! D41   D(22,11,13,16)  -179.0918  178.8408 -177.9761 -DE/DX =    0.0         !
```

```
! D42   D(22,11,13,17)    0.9741   -0.7569    1.9184 -DE/DX =    0.0         !
! D43   D(12,11,22,23)   -60.8858  -68.1041  -53.4485 -DE/DX =    0.0         !
! D44   D(12,11,22,25)   170.1963  174.4053  170.5089 -DE/DX =    0.0         !
! D45   D(12,11,22,28)    72.2164   72.2707   68.4321 -DE/DX =    0.0         !
! D46   D(13,11,22,23)   118.2984  112.47    124.454  -DE/DX =    0.0         !
! D47   D(13,11,22,25)   -10.6194   -5.0205  -11.5886 -DE/DX =    0.0         !
! D48   D(13,11,22,28)  -108.5994 -107.1552 -113.6655 -DE/DX =    0.0         !
! D49   D(11,12,14,18)    -0.0091   -0.123    -0.1034 -DE/DX =    0.0         !
! D50   D(11,12,14,19)   179.9032  179.5575  179.932  -DE/DX =    0.0         !
! D51   D(15,12,14,18)  -179.9376 -179.4301  179.6012 -DE/DX =    0.0         !
! D52   D(15,12,14,19)    -0.0253    0.2505   -0.3634 -DE/DX =    0.0         !
! D53   D(11,13,16,18)    -0.1107    0.1818   -0.1063 -DE/DX =    0.0         !
! D54   D(11,13,16,20)   179.8903 -179.6913  179.8388 -DE/DX =    0.0         !
! D55   D(17,13,16,18)   179.8227  179.7789 -179.9985 -DE/DX =    0.0         !
! D56   D(17,13,16,20)    -0.1763   -0.0941   -0.0534 -DE/DX =    0.0         !
! D57   D(12,14,18,16)     0.0041   -0.2962    0.034  -DE/DX =    0.0         !
! D58   D(12,14,18,21)   179.9221  179.6398 -179.9953 -DE/DX =    0.0         !
! D59   D(19,14,18,16)  -179.9083 -179.9766  179.9987 -DE/DX =    0.0         !
! D60   D(19,14,18,21)     0.0097   -0.0406   -0.0306 -DE/DX =    0.0         !
! D61   D(13,16,18,14)     0.0548    0.2679    0.0688 -DE/DX =    0.0         !
! D62   D(13,16,18,21)  -179.8631 -179.6681 -179.9019 -DE/DX =    0.0         !
! D63   D(20,16,18,14)  -179.9462 -179.859  -179.8764 -DE/DX =    0.0         !
! D64   D(20,16,18,21)    0.1359    0.205     0.1529 -DE/DX =    0.0         !
! D65   D(11,22,23,24)   -16.4756  -11.7998  -22.8783 -DE/DX =    0.0         !
! D66   D(25,22,23,24)   111.6758  106.0071  111.8683 -DE/DX =    0.0         !
! D67   D(28,22,23,24)  -149.4022 -151.5889 -144.76   -DE/DX =    0.0         !
! D68   D(11,22,25,26)   146.8254  146.5458  150.2655 -DE/DX =    0.0         !
! D69   D(11,22,25,27)  -113.7625 -111.3884 -110.6896 -DE/DX =    0.0         !
! D70   D(23,22,25,26)    14.8206   22.1012   14.6371 -DE/DX =    0.0         !
! D71   D(23,22,25,27)   114.2327  124.167   113.682  -DE/DX =    0.0         !
! D72   D(28,22,25,26)   -99.5182  -96.3966  -97.9063 -DE/DX =    0.0         !
! D73   D(28,22,25,27)    -0.1062    5.6692    1.1386 -DE/DX =    0.0         !
! D74   D(11,22,28,1)   -134.2419 -139.9068 -131.8522 -DE/DX =    0.0         !
! D75   D(11,22,28,27)   111.5244  106.8008  113.6542 -DE/DX =    0.0         !
! D76   D(11,22,28,32)     3.4156   -0.037     5.3996 -DE/DX =    0.0         !
! D77   D(23,22,28,1)      1.0757    0.628    -6.1718 -DE/DX =    0.0         !
! D78   D(23,22,28,27)  -113.1581 -112.6644 -120.6654 -DE/DX =    0.0         !
! D79   D(23,22,28,32)   138.7332  140.4978  131.08   -DE/DX =    0.0         !
! D80   D(25,22,28,1)    114.3297  110.2113  112.5532 -DE/DX =    0.0         !
! D81   D(25,22,28,27)     0.0959   -3.0811   -1.9405 -DE/DX =    0.0         !
! D82   D(25,22,28,32)  -108.0128 -109.9189 -110.195  -DE/DX =    0.0         !
! D83   D(22,25,27,28)     0.1606   -4.6648   -1.9307 -DE/DX =    0.0         !
! D84   D(26,25,27,28)   105.4645   99.0983  104.4053 -DE/DX =    0.0         !
! D85   D(25,27,28,1)   -121.9343 -116.8724 -128.0983 -DE/DX =    0.0         !
! D86   D(25,27,28,22)    -0.1645    5.7756    1.6177 -DE/DX =    0.0         !
! D87   D(25,27,28,32)   104.2813  111.3114  112.3136 -DE/DX =    0.0         !
```

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
%nprocshared=3
Will use up to 3 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\IRC work\FREQ-QS
T2-BDAB-OBTAINED FROM IRC2-PRODUCT FORMATION.chk
---
freq wb97xd/6-31g(d,p)

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.261714 (Hartree/Particle)
Thermal correction to Energy= 0.276593
Thermal correction to Enthalpy= 0.277538
Thermal correction to Gibbs Free Energy= 0.219099
Sum of electronic and zero-point Energies= -750.713719
Sum of electronic and thermal Energies= -750.698840
Sum of electronic and thermal Enthalpies= -750.697895
Sum of electronic and thermal Free Energies= -750.756334

METHOD VALIDATION

LOWEST ENERGY CONFORMATION FOR 3.7

3.7A
%nprocshared=3
Will use up to 3 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\Intermediates\OP
T-FREQ-INT A using INT C.chk
---
opt freq wb97xd/6-31g(d,p)

1/14=-1,18=20,19=15,26=3,38=1/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4//1;
5/5=2,38=5/2;

6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(2);
2/9=110/2;
99//99;
2/9=110/2;
3/5=1,6=6,7=101,11=2,16=1,25=1,30=1,71=1,74=-58/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	1.6995	-0.37755	0.10272
C	2.558	0.69992	0.36042
C	3.9303	0.55192	0.18069
C	4.45744	-0.66282	-0.24647
C	3.6101	-1.73657	-0.4988
C	2.23867	-1.58866	-0.31961
H	4.58622	1.39461	0.38152
H	5.52874	-0.76359	-0.38111
H	4.01148	-2.68683	-0.83299
H	1.55401	-2.40975	-0.50325
C	-2.08433	0.13384	-0.06274
C	-3.11214	1.01985	-0.41484
C	-2.44202	-1.14782	0.37822
C	-4.44911	0.64301	-0.33037
H	-2.85587	2.01798	-0.75831
C	-3.77662	-1.53224	0.46735
H	-1.66159	-1.85042	0.65563
C	-4.78237	-0.6355	0.11246
H	-5.23064	1.34371	-0.6076
H	-4.03378	-2.52909	0.81241
H	-5.82466	-0.93192	0.18252
O	0.34995	-0.32561	0.31183
B	-0.58442	0.57912	-0.16406
O	-0.28336	1.78714	-0.70274
H	0.61151	2.07725	-0.47354
N	1.95087	1.96307	0.80401
H	2.09518	2.07508	1.78718

H 2.37458 2.72607 0.31585

GradGradGradG

---
opt freq wb97xd/6-31g(d,p)

Zero-point correction= 0.213112 (Hartree/Particle)
Thermal correction to Energy= 0.226380
Thermal correction to Enthalpy= 0.227324
Thermal correction to Gibbs Free Energy= 0.170998
Sum of electronic and zero-point Energies= -714.101407
Sum of electronic and thermal Energies= -714.088139
Sum of electronic and thermal Enthalpies= -714.087195
Sum of electronic and thermal Free Energies= -714.143521

3.7D

%nprocshared=2
Will use up to 2 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\Intermediates\Using INT C\INT D by C.chk
---
opt freq wb97xd/6-31g(d,p)

Zero-point correction= 0.239644 (Hartree/Particle)
Thermal correction to Energy= 0.252964
Thermal correction to Enthalpy= 0.253909
Thermal correction to Gibbs Free Energy= 0.198727
Sum of electronic and zero-point Energies= -674.358339
Sum of electronic and thermal Energies= -674.345019
Sum of electronic and thermal Enthalpies= -674.344074
Sum of electronic and thermal Free Energies= -674.399256

CHAPTER 2 – COMPUTATIONAL OUTPUT FILES

Using b3lyp/6-311+g method

1. Benzoxazaborole 2.1

%nprocshared=2
Will use up to 2 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\CH2\heteroborole
-Default-CHCl3+ basis set\Gas phase\OPT-FREQ-BOAB-NORTHROPE-Gas phase9-4.chk

---
opt freq b3lyp/6-311+g(d,p)

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.196190 (Hartree/Particle)
Thermal correction to Energy= 0.207328
Thermal correction to Enthalpy= 0.208272
Thermal correction to Gibbs Free Energy= 0.157878
Sum of electronic and zero-point Energies= -618.200109
Sum of electronic and thermal Energies= -618.188971
Sum of electronic and thermal Enthalpies= -618.188027
Sum of electronic and thermal Free Energies= -618.238421

2. Benzodioxaborole 2.3

%nprocshared=3
Will use up to 3 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\CH2\heteroborole
-Default-CHCl3+ basis set\Gas phase\OPT-FREQ-NORTHROPE-BDOB-Gas phase-9-4.chk
---
opt freq b3lyp/6-311+g(d,p)

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.183837 (Hartree/Particle)
Thermal correction to Energy= 0.194709
Thermal correction to Enthalpy= 0.195653
Thermal correction to Gibbs Free Energy= 0.145964
Sum of electronic and zero-point Energies= -638.087934
Sum of electronic and thermal Energies= -638.077062
Sum of electronic and thermal Enthalpies= -638.076118
Sum of electronic and thermal Free Energies= -638.125806

3. Benzodiazaborole 2.6

%nprocshared=2

Will use up to 2 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\CH2\heteroborole -Default-CHCl3+ basis set\Gas phase\OPT-FREQ-BDAB-NORTHROPE-DEFAULT-Gas phase-9-4.chk
---
opt freq b3lyp/6-311+g(d,p)

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.208632 (Hartree/Particle)
Thermal correction to Energy= 0.220011
Thermal correction to Enthalpy= 0.220955
Thermal correction to Gibbs Free Energy= 0.170169
Sum of electronic and zero-point Energies= -598.311973
Sum of electronic and thermal Energies= -598.300595
Sum of electronic and thermal Enthalpies= -598.299651
Sum of electronic and thermal Free Energies= -598.350437

4. Ethyl benzoxazaborole 2.8

%nprocshared=3
Will use up to 3 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\CH2\heteroborole -Default-CHCl3+ basis set\Gas phase\OPT-FREQ-NORTHROPE-ETH BOAB-Gas phase-9-4.ch k
---
opt freq b3lyp/6-311+g(d,p)

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.252561 (Hartree/Particle)
Thermal correction to Energy= 0.266499
Thermal correction to Enthalpy= 0.267443
Thermal correction to Gibbs Free Energy= 0.211026
Sum of electronic and zero-point Energies= -696.784935

Sum of electronic and thermal Energies= -696.770997
Sum of electronic and thermal Enthalpies= -696.770053
Sum of electronic and thermal Free Energies= -696.826470

using b3lyp/6-311+g(d,p) basis set

1. **Benzoxazaborole 2.1**

%nprocshared=2
Will use up to 2 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\CH2\heteroborole
-Default-CHCl3+ basis set\OPT-FREQ-BOAB-NORTHROPE-DEFAULT-CHCL3-9-4.chk
---
opt freq b3lyp/6-311+g(d,p) scrf=(solvent=chloroform)

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.196063 (Hartree/Particle)
Thermal correction to Energy= 0.207241
Thermal correction to Enthalpy= 0.208185
Thermal correction to Gibbs Free Energy= 0.156797
Sum of electronic and zero-point Energies= -618.205641
Sum of electronic and thermal Energies= -618.194464
Sum of electronic and thermal Enthalpies= -618.193520
Sum of electronic and thermal Free Energies= -618.244908

2. **Benzodioxaborole 2.3**

%nprocshared=3
Will use up to 3 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\CH2\heteroborole

-Default-CHCl3+ basis set\OPT-FREQ-NORTHROPE-BDOB-DEFAULT-CHCL3-9-4.chk
---
opt freq b3lyp/6-311+g(d,p) scrf=(solvent=chloroform)

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.183647 (Hartree/Particle)
Thermal correction to Energy= 0.194546
Thermal correction to Enthalpy= 0.195490
Thermal correction to Gibbs Free Energy= 0.145656
Sum of electronic and zero-point Energies= -638.091816
Sum of electronic and thermal Energies= -638.080917
Sum of electronic and thermal Enthalpies= -638.079973
Sum of electronic and thermal Free Energies= -638.129807

3. **Benzodiazaborole 2.6**

%nprocshared=2
Will use up to 2 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\CH2\heteroborole
-Default-CHCl3+ basis set\OPT-FREQ-BDAB-NORTHROPE-DEFAULT-CHCL3-9-4.chk
---
opt freq b3lyp/6-311+g(d,p) scrf=(solvent=chloroform)

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.208614 (Hartree/Particle)
Thermal correction to Energy= 0.219985
Thermal correction to Enthalpy= 0.220929
Thermal correction to Gibbs Free Energy= 0.169920
Sum of electronic and zero-point Energies= -598.318219
Sum of electronic and thermal Energies= -598.306849
Sum of electronic and thermal Enthalpies= -598.305905
Sum of electronic and thermal Free Energies= -598.356914

4. **Ethyl benzoxazaborole 2.8**

%nprocshared=3
Will use up to 3 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\OPT-ETH BOAB-Nor
thrope-Default-~~Gas phase~~.chk
---
opt freq b3lyp/6-311+g(d,p) scrf=(solvent=chloroform)

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.252374 (Hartree/Particle)
Thermal correction to Energy= 0.266338
Thermal correction to Enthalpy= 0.267282
Thermal correction to Gibbs Free Energy= 0.210756
Sum of electronic and zero-point Energies= -696.789662
Sum of electronic and thermal Energies= -696.775698
Sum of electronic and thermal Enthalpies= -696.774754
Sum of electronic and thermal Free Energies= -696.831280

Donor molecules

1. Catechol 2.2

%nprocshared=3
Will use up to 3 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\CH2\donor molecu
le\Gas phase\OPT-FREQ-CAT-NORTHROPE-Gasphase-9-4-From-TRIAL 3.chk
---
opt freq b3lyp/6-311+g(d,p)

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.108291 (Hartree/Particle)
Thermal correction to Energy= 0.115193
Thermal correction to Enthalpy= 0.116138
Thermal correction to Gibbs Free Energy= 0.077544
Sum of electronic and zero-point Energies= -382.698687
Sum of electronic and thermal Energies= -382.691785
Sum of electronic and thermal Enthalpies= -382.690841
Sum of electronic and thermal Free Energies= -382.729434

2. 2-aminophenol 2.4

%nprocshared=3

Will use up to 3 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\CH2\donor molecule\OPT-FREQ-OAP-Northrope-NH2 donating to H- confor-Gas phase.chk
---
opt freq b3lyp/6-311+g(d,p)

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.121341 (Hartree/Particle)
Thermal correction to Energy= 0.128359
Thermal correction to Enthalpy= 0.129303
Thermal correction to Gibbs Free Energy= 0.089329
Sum of electronic and zero-point Energies= -362.813296
Sum of electronic and thermal Energies= -362.806279
Sum of electronic and thermal Enthalpies= -362.805334
Sum of electronic and thermal Free Energies= -362.845308

3. Benzene-1,2-diamine 2.5

%nprocshared=2
Will use up to 2 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\CH2\donor molecule\Gas phase\OPT-FREQ-OPD-NORTHROPE-Gas phase-9-4.chk
---
opt freq b3lyp/6-311+g(d,p)

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.133951 (Hartree/Particle)
Thermal correction to Energy= 0.140995
Thermal correction to Enthalpy= 0.141939
Thermal correction to Gibbs Free Energy= 0.103289
Sum of electronic and zero-point Energies= -342.929701
Sum of electronic and thermal Energies= -342.922657
Sum of electronic and thermal Enthalpies= -342.921713
Sum of electronic and thermal Free Energies= -342.960362

4. Ethyl aminophenol 2.8

%nprocshared=3

Will use up to 3 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\CH2\donor molecu
le\Gas phase\OPT-FREQ-ETH OAP-NORTHROPE-Gas phase-9-4-T2.chk
---
opt freq b3lyp/6-311+g(d,p)

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.177991 (Hartree/Particle)
Thermal correction to Energy= 0.187456
Thermal correction to Enthalpy= 0.188400
Thermal correction to Gibbs Free Energy= 0.142799
Sum of electronic and zero-point Energies= -441.398059
Sum of electronic and thermal Energies= -441.388594
Sum of electronic and thermal Enthalpies= -441.387650
Sum of electronic and thermal Free Energies= -441.433251

1. Catechol 2.2

%chk=C:\Users\thush\Searches\CAT-Northrope

basis set-Default-CHCl3-OH bonded.chk
---
opt freq b3lyp/6-311+g(d,p) scrf=(solvent=chloroform)

1/18=20,19=15,26=3,38=1/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=4,6=6,7=111,11=2,25=1,30=1,70=2201,71=1,72=7,74=-5/1,2,3;
4//1;
5/5=2,38=5,53=7/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/18=20,19=15,26=3/3(2);
2/9=110/2;
99//99;
2/9=110/2;
3/5=4,6=6,7=111,11=2,25=1,30=1,70=2205,71=1,72=7,74=-5/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5,53=7/2;
7//1,2,3,16;
1/18=20,19=15,26=3/3(-5);
2/9=110/2;

6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C							
C	1	B1					
C	2	B2	1	A1			
C	3	B3	2	A2	1	D1	0
C	4	B4	3	A3	2	D2	0
C	1	B5	2	A4	3	D3	0
H	1	B6	6	A5	5	D4	0
H	2	B7	1	A6	6	D5	0
H	5	B8	4	A7	3	D6	0
H	6	B9	1	A8	2	D7	0
O	3	B10	2	A9	1	D8	0
O	4	B11	3	A10	2	D9	0
H	12	B12	4	A11	3	D10	0
H	11	B13	3	A12	2	D11	0

Variables:

B1	1.4014
B2	1.4014
B3	1.4014
B4	1.4014
B5	1.4014
B6	1.07
B7	1.07
B8	1.07
B9	1.07
B10	1.43
B11	1.43
B12	0.96
B13	0.96
A1	120.
A2	120.
A3	120.
A4	120.
A5	120.
A6	120.
A7	120.
A8	120.
A9	120.
A10	120.
A11	109.47122

A12 109.47122
D1 0.
D2 0.
D3 0.
D4 180.
D5 -180.
D6 180.
D7 180.
D8 -180.
D9 180.
D10 -150.
D11 -120.9754

2 tetrahedral angles replaced.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.
Initialization pass.

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.108254 (Hartree/Particle)
Thermal correction to Energy= 0.115052
Thermal correction to Enthalpy= 0.115996
Thermal correction to Gibbs Free Energy= 0.077702
Sum of electronic and zero-point Energies= -382.704678
Sum of electronic and thermal Energies= -382.697880
Sum of electronic and thermal Enthalpies= -382.696936
Sum of electronic and thermal Free Energies= -382.735230

2. 2-aminophenol 2.4

%chk=C:\Users\thush\Searches\OPT-FREQ-OAP-Northrope basis set-Default-CHCl3-NH2-Sp2-conjugated with ph-no H bonding of OH.chk
---
opt freq b3lyp/6-311+g(d,p) scrf=(solvent=chloroform)

1/18=20,19=15,26=3,38=1/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=4,6=6,7=111,11=2,25=1,30=1,70=2201,71=1,72=7,74=-5/1,2,3;
4//1;
5/5=2,38=5,53=7/2;
6/7=2,8=2,9=2,10=2,28=1/1;

```
7//1,2,3,16;
1/18=20,19=15,26=3/3(2);
2/9=110/2;
99//99;
2/9=110/2;
3/5=4,6=6,7=111,11=2,25=1,30=1,70=2205,71=1,72=7,74=-5/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5,53=7/2;
7//1,2,3,16;
1/18=20,19=15,26=3/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;
---
Title Card Required
---
Symbolic Z-matrix:
Charge =  0 Multiplicity = 1
C
C                  1    B1
C                  2    B2      1    A1
C                  3    B3      2    A2      1    D1      0
C                  4    B4      3    A3      2    D2      0
C                  1    B5      2    A4      3    D3      0
H                  1    B6      6    A5      5    D4      0
H                  2    B7      1    A6      6    D5      0
H                  5    B8      4    A7      3    D6      0
H                  6    B9      1    A8      2    D7      0
N                  4    B10     3    A9      2    D8      0
H                  11   B11     4    A10     3    D9      0
H                  11   B12     4    A11     3    D10     0
O                  3    B13     2    A12     1    D11     0
H                  14   B14     3    A13     2    D12     0
     Variables:
 B1                1.39896
 B2                1.38751
 B3                1.4113
 B4                1.40106
 B5                1.39198
 B6                1.08327
 B7                1.08628
 B8                1.08528
 B9                1.0841
 B10               1.37669
 B11               1.00445
 B12               1.00425
```

B13	1.37907
B14	0.96353
A1	120.41082
A2	121.014
A3	117.85098
A4	119.2449
A5	120.8642
A6	120.29784
A7	118.82763
A8	120.2665
A9	119.39208
A10	120.24133
A11	121.03136
A12	123.47564
A13	110.04158
D1	0.00053
D2	-0.00153
D3	0.
D4	-179.99954
D5	-179.99922
D6	-180.
D7	179.99941
D8	179.98696
D9	0.13527
D10	179.87242
D11	-179.99916
D12	0.00947

GradGradGradG

3. Benzene-1,2-diamine 2.5

%nprocshared=2
Will use up to 2 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\CH2\donor molecule\OPT-FREQ-OPD-NORTHROPE-DEFAULT-CHCL3-9-4.chk
---
opt freq b3lyp/6-311+g(d,p) scrf=(solvent=chloroform)

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.133806 (Hartree/Particle)
Thermal correction to Energy= 0.140851
Thermal correction to Enthalpy= 0.141795
Thermal correction to Gibbs Free Energy= 0.103162
Sum of electronic and zero-point Energies= -342.936039
Sum of electronic and thermal Energies= -342.928994
Sum of electronic and thermal Enthalpies= -342.928050
Sum of electronic and thermal Free Energies= -342.966683

4. Ethyl aminophenol 2.7

%nprocshared=3
Will use up to 3 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\CH2\donor molecu
le\OPT-FREQ-Eth OAP-NORTHROPE-DEFAULT-CHCL3-9-4.chk
---
opt freq b3lyp/6-311+g(d,p) scrf=(solvent=chloroform)

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.177742 (Hartree/Particle)
Thermal correction to Energy= 0.187216
Thermal correction to Enthalpy= 0.188161
Thermal correction to Gibbs Free Energy= 0.142593
Sum of electronic and zero-point Energies= -441.402940
Sum of electronic and thermal Energies= -441.393466
Sum of electronic and thermal Enthalpies= -441.392522
Sum of electronic and thermal Free Energies= -441.438089

Using b3lyp/6-311++g(d,p) method

Benzodiazaborole in $CHCl_3$ 2.6

%nprocshared=2
Will use up to 2 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\CH2\OPT-FREQ-BDA
B-CRR-Default-CHCl3.chk
---
opt freq b3lyp/6-311++g(d,p) scrf=(solvent=chloroform)

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.208602 (Hartree/Particle)
Thermal correction to Energy= 0.219962
Thermal correction to Enthalpy= 0.220906
Thermal correction to Gibbs Free Energy= 0.170061
Sum of electronic and zero-point Energies= -598.318338
Sum of electronic and thermal Energies= -598.306979
Sum of electronic and thermal Enthalpies= -598.306034
Sum of electronic and thermal Free Energies= -598.356880

Gas phase

nprocshared=3
Will use up to 3 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\CH2\OPT-FREQ-BDA
B-CRR-Gas phase-T2.chk
---
opt freq b3lyp/6-311++g(d,p)

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.208582 (Hartree/Particle)
Thermal correction to Energy= 0.219963
Thermal correction to Enthalpy= 0.220907
Thermal correction to Gibbs Free Energy= 0.170107

Sum of electronic and zero-point Energies= -598.312132
Sum of electronic and thermal Energies= -598.300750
Sum of electronic and thermal Enthalpies= -598.299806
Sum of electronic and thermal Free Energies= -598.350606

Benzodioxaborole 2.3

%nprocshared=3
Will use up to 3 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\CH2\OPT-FREQ-BDO
B-CRR-Default-CHCl3.chk
---
opt freq b3lyp/6-311++g(d,p) scrf=(solvent=chloroform)

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.Zero-point correction= 0.183613 (Hartree/Particle)
Thermal correction to Energy= 0.194514
Thermal correction to Enthalpy= 0.195458
Thermal correction to Gibbs Free Energy= 0.145615
Sum of electronic and zero-point Energies= -638.091933
Sum of electronic and thermal Energies= -638.081032
Sum of electronic and thermal Enthalpies= -638.080088
Sum of electronic and thermal Free Energies= -638.129931

Gas phase

%nprocshared=3
Will use up to 3 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\CH2\OPT-FREQ-BDO
B-CRR-Gas phasef.chk
---
opt freq b3lyp/6-311++g(d,p)

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.183783 (Hartree/Particle)

Thermal correction to Energy= 0.194658
Thermal correction to Enthalpy= 0.195602
Thermal correction to Gibbs Free Energy= 0.145907
Sum of electronic and zero-point Energies= -638.088072
Sum of electronic and thermal Energies= -638.077197
Sum of electronic and thermal Enthalpies= -638.076253
Sum of electronic and thermal Free Energies= -638.125948

Benoxazaborole 2.1

%nprocshared=2
Will use up to 2 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\CH2\OPT-FREQ-BOA
B-CRR-Default-CHCl3.chk
---
opt freq b3lyp/6-311++g(d,p) scrf=(solvent=chloroform)

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Atom 1 has atomic number 6 and mass 12.00000
Zero-point correction= 0.196027 (Hartree/Particle)
Thermal correction to Energy= 0.207206
Thermal correction to Enthalpy= 0.208150
Thermal correction to Gibbs Free Energy= 0.156800
Sum of electronic and zero-point Energies= -618.205774
Sum of electronic and thermal Energies= -618.194596
Sum of electronic and thermal Enthalpies= -618.193652
Sum of electronic and thermal Free Energies= -618.245002

Gas phase

%nprocshared=2
Will use up to 2 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\CH2\OPT-FREQ-BOA
B-CRR-Gas phase.chk

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

---
opt freq b3lyp/6-311++g(d,p)

Zero-point correction= 0.196131 (Hartree/Particle)
Thermal correction to Energy= 0.207272
Thermal correction to Enthalpy= 0.208217
Thermal correction to Gibbs Free Energy= 0.157818
Sum of electronic and zero-point Energies= -618.200267
Sum of electronic and thermal Energies= -618.189125
Sum of electronic and thermal Enthalpies= -618.188181
Sum of electronic and thermal Free Energies= -618.238580

Ethyl benzoxazaborole 2.8

%nprocshared=3
Will use up to 3 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\CH2\OPT-FREQ-Eth
BOAB-CRR-Default-CHCl3.chk
---
opt freq b3lyp/6-311++g(d,p) scrf=(solvent=chloroform)

- Thermochemistry -
Zero-point correction= 0.252337 (Hartree/Particle)
Thermal correction to Energy= 0.266301
Thermal correction to Enthalpy= 0.267246
Thermal correction to Gibbs Free Energy= 0.210718
Sum of electronic and zero-point Energies= -696.789837
Sum of electronic and thermal Energies= -696.775872
Sum of electronic and thermal Enthalpies= -696.774928
Sum of electronic and thermal Free Energies= -696.831456

%nprocshared=3
Will use up to 3 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\CH2\OPT-FREQ-Eth
BOAB-CRR-Gas phasef.chk
---
opt freq b3lyp/6-311++g(d,p)

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.252505 (Hartree/Particle)
Thermal correction to Energy= 0.266446
Thermal correction to Enthalpy= 0.267391
Thermal correction to Gibbs Free Energy= 0.210962
Sum of electronic and zero-point Energies= -696.785132
Sum of electronic and thermal Energies= -696.771191
Sum of electronic and thermal Enthalpies= -696.770247
Sum of electronic and thermal Free Energies= -696.826675

Ethyl aminophenol 2.7

%nprocshared=4
Will use up to 4 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\CH2\donor molecu
le\OPT-FREQ-ETH OAP-CRR-H bonding confor-Default-CHCl3.chk
---
opt freq b3lyp/6-311++g(d,p) scrf=(solvent=chloroform)

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.177719 (Hartree/Particle)
Thermal correction to Energy= 0.187195
Thermal correction to Enthalpy= 0.188139
Thermal correction to Gibbs Free Energy= 0.142563
Sum of electronic and zero-point Energies= -441.403113
Sum of electronic and thermal Energies= -441.393637
Sum of electronic and thermal Enthalpies= -441.392693
Sum of electronic and thermal Free Energies= -441.438269

%nprocshared=4
Will use up to 4 processors via shared memory.
%mem=1GB
%chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\CH2\donor molecu
le\OPT-FREQ-ETH OAP-CRR-H bonding confor-Gas phase.chk
---
opt freq b3lyp/6-311++g(d,p)

 - Thermochemistry -

Zero-point correction= 0.177963 (Hartree/Particle)
 Thermal correction to Energy= 0.187430
 Thermal correction to Enthalpy= 0.188375
 Thermal correction to Gibbs Free Energy= 0.142763
 Sum of electronic and zero-point Energies= -441.398243
 Sum of electronic and thermal Energies= -441.388776
 Sum of electronic and thermal Enthalpies= -441.387831
 Sum of electronic and thermal Free Energies= -441.433443

2-aminophenol 2.4

%nprocshared=3
 Will use up to 3 processors via shared memory.
 %mem=1GB
 %chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\CH2\donor molecu
 le\OPT-FREQ-OAP-CRR-NH2 donating to H- confor-Gas phase.chk

 # opt freq b3lyp/6-311++g(d,p)

 - Thermochemistry -

 Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.121315 (Hartree/Particle)
 Thermal correction to Energy= 0.128343
 Thermal correction to Enthalpy= 0.129287
 Thermal correction to Gibbs Free Energy= 0.089133
 Sum of electronic and zero-point Energies= -362.813444
 Sum of electronic and thermal Energies= -362.806416
 Sum of electronic and thermal Enthalpies= -362.805472
 Sum of electronic and thermal Free Energies= -362.845626

Benzene-1,2-diamine 2.5

%nprocshared=2
 Will use up to 2 processors via shared memory.
 %mem=1GB
 %chk=T:\CHM\deg013\Thushini\Reproducing data of li et. al paper\CRR basis set-de
 fault solvent model\FREQ-OPD-CRR BASIS SET.chk

 # freq b3lyp/6-311++g(d,p) scrf=(solvent=chloroform)

- Thermochemistry -

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.133791 (Hartree/Particle)
Thermal correction to Energy= 0.140836
Thermal correction to Enthalpy= 0.141780
Thermal correction to Gibbs Free Energy= 0.103147
Sum of electronic and zero-point Energies= -342.936191
Sum of electronic and thermal Energies= -342.929146
Sum of electronic and thermal Enthalpies= -342.928202
Sum of electronic and thermal Free Energies= -342.966835

Catechol 2.2

%chk=C:\Users\thush\Searches\CAT-CRR basis set-Default-CHCl3-OH bonded.chk
---
opt freq b3lyp/6-311++g(d,p) scrf=(solvent=chloroform)

1/18=20,19=15,26=3,38=1/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=4,6=6,7=1111,11=2,25=1,30=1,70=2201,71=1,72=7,74=-5/1,2,3;
4//1;
5/5=2,38=5,53=7/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/18=20,19=15,26=3/3(2);
2/9=110/2;
99//99;
2/9=110/2;
3/5=4,6=6,7=1111,11=2,25=1,30=1,70=2205,71=1,72=7,74=-5/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5,53=7/2;
7//1,2,3,16;
1/18=20,19=15,26=3/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;

Title Card Required

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1
C

```
C                1   B1
C                2   B2      1   A1
C                3   B3      2   A2      1   D1      0
C                4   B4      3   A3      2   D2      0
C                1   B5      2   A4      3   D3      0
H                1   B6      6   A5      5   D4      0
H                2   B7      1   A6      6   D5      0
H                5   B8      4   A7      3   D6      0
H                6   B9      1   A8      2   D7      0
O                3   B10     2   A9      1   D8      0
O                4   B11     3   A10     2   D9      0
H               12   B12     4   A11     3   D10     0
H               11   B13     3   A12     2   D11     0
     Variables:
 B1               1.4014
 B2               1.4014
 B3               1.4014
 B4               1.4014
 B5               1.4014
 B6               1.07
 B7               1.07
 B8               1.07
 B9               1.07
 B10              1.43
 B11              1.43
 B12              0.96
 B13              0.96
 A1              120.
 A2              120.
 A3              120.
 A4              120.
 A5              120.
 A6              120.
 A7              120.
 A8              120.
 A9              120.
 A10              120.
 A11              109.47122
 A12              109.47122
 D1               0.
 D2               0.
 D3               0.
 D4              180.
 D5             -180.
 D6              180.
 D7              180.
```

D8 -180.
D9 180.
D10 -150.
D11 -120.9754

2 tetrahedral angles replaced.

GradGradGradG

VITA

EDUCATION

MS	Sam Houston State University	August 2018 – Present
	Chemistry	3.77/4.00
	Research area	Organic chemistry
	Advisor	Dr. Dustin E. Gross
BS	University of Peradeniya	2014
	Applied Sciences	3.30/4.00
	Chemistry and Botany (Joint Major)	
	Research area	Analytical chemistry
	Advisor	Dr. Rupika Rajakaruna

FELLOWSHIPS & AWARDS

ACS PRF Research Fellowship (Summer 2020)

Robert A. Welch Research Fellowship (Summer 2019, Summer 2021)

Graduate Achievement Scholarship: College of Science and Engineering (Academic year 2018- 2020)

TEACHING EXPERIENCE

2018- 2021 SAM HOUSTON STATE UNIVERSITY Huntsville, TX
Teaching Assistant, Department of Chemistry
(Lab: 15-30 students)
Responsibilities: conducted lab sessions, supervised students in the lab, held tutoring hours, graded exams and lab reports, examination proctoring.

2018 Fall	Organic chemistry I laboratory	Dr. Dustin E. Gross
2019 Spring	Organic chemistry I laboratory	Dr. Dustin E. Gross
2019-2020	General Chemistry II laboratory	Dr. Christopher M. Zall Steven Hegwood, MS
	Inorganic and environmental chemistry	Dr. Melanie Rose
2020 Fall	Quantitative Analysis	Dr. Tarek Trad
2021 Spring	Quantitative Analysis	Dr. David E. Thompson
2021 Fall	Quantitative Analysis	Dr. Tarek Trad
	General Chemistry II laboratory	Dr. Christopher M. Zall

2014 – 2015 University of Rajarata, Sri Lanka
Teaching Assistant, Department of Physical Sciences, Faculty of Applied Sciences
(Lab: 30-40 students)

Responsibilities: conducted chemistry laboratory sessions, helped to develop lab experiments, supervised students in the lab, graded exams, and lab reports, and examination proctoring.

2014 Fall	Inorganic chemistry laboratory	Dr. H.M.A. Herath
	Analytical chemistry laboratory	Dr. H.M.A. Herath
2015 Spring	Organic chemistry laboratory	Dr. E.M. Edirisinghe

CONFERENCE AND SYMPOSIUM PRESENTATIONS

Hemachandra, T. P.; Gross D. E. Solution phase and computational studies on the formation, hydrolysis, and dynamic exchange of phenyl benzoboroles. the American Chemical Society, El Paso, TX, United States, April 01-30, 2021.
(through Zoom).

Hemachandra, T. P.; Gross D. E. Determination of relative stability of heteroborole systems using dynamic covalent reactions. Texas Academy of Science**,** Stephen F. Austin State University in Nacogdoches, TX, February 28-29, 2020.

Hemachandra, T. P.; Rathnayaka, R. M. C.;Gross, D. E. Thermodynamic and kinetic studies of dynamic covalent reactions involving benzoxazaboroles. Published in Abstracts, 75th Southwest Regional Meeting of the American Chemical Society, El Paso, TX, United States, November 13-15 2019.

Jayewardena, W. J. C. M.; Hemachandra T.P.; Thiruchenduran S.; Ganegama Arachchi G. J.; Rajapakse R. P. N. P. An Assessment of heavy metals and *Escherichia coli* contamination of selected seaweeds collected from southern coastal area of Sri Lanka Published in the proceedings of the NARA International Scientific Sessions in July 2018.

Hemachandra, T.P.; Jayewardena W. J. C. M.; Thiruchenduran S.; Ganegama Arachchi G. J.; Rajapakse R. P. N. P. Determination of proximate and mineral composition of *Ulva reticulata, Caulerpa racemosa* and *Sargassum Wightii* in southern coast of Sri Lanka. Published in the proceedings of the NARA International Scientific Sessions in July 2018

Hemachandra, T.P.; Jayathilake R.R.G.D.K, Madhujith T. The effect of selected plant extracts in reducing oxidation of selected edible oils during deep frying. Published in the proceedings of the Peradeniya University International Research Sessions in November 2016.

Jayahilake, R.R.G.D.K.; Hemachandra T.P.; Madhujith, T. The effect of selected plant extracts in reducing autoxidation of selected edible oils during storage. Published in the proceedings of the Peradeniya University International Research Sessions in November 2016.

Hemachandra, T.P.; Jayathilake R.R.G.D.K.; Madhujith T. (2016). The effect of Antioxidative Extracts in Reducing Oxidation of Selected Edible Oils during Deep Frying. Tropical Agricultural Research, Volume 28.

INSTRUMENTATIONS AND SKILLS

Lab techniques – Schlenk techniques, Organic synthesis and characterization

Instrumentation – NMR, GC, HPLC, UV-vis and fluorescence spectroscopy, atomic absorption spectroscopy

Software – ChemDraw, Gaussian 9.0, Mendeley, MS-office, SciFinder, Adobe.

COLLABORATIVE WORK

- Collaborative research project with Sri Lanka Atomic Energy Board, Colombo for Detecting of Radioactive Residue in Marine consumable fish. January-July, 2018.

- Database management and collaborative work on ecosystem survey for NANSEN Program/FAO/UN on Norwegian Research Vessel Dr. Fridj of Nansen in Sri Lanka. March-July 2018.

WORK EXPERIENCES

2016 December—2018 July: Research officer: national aquatic resources research & development agency (NARA).
Responsibilities: overall management of the laboratory, continuation of group research projects on bioactive ingredients of the marine resources mainly seaweeds, assisting undergraduates on their research projects.

2015 August—2016 May: Research assistant, faculty of agriculture, university of Peradeniya.
Responsibilities: continuation of group research projects on antioxidants and oil oxidation, assisting undergraduates on their research projects, purchase of chemicals and equipment.

2014 May—2015 May: Teaching assistant, faculty of applied sciences, university of Rajarata.
Responsibilities: conducting chemistry laboratory sessions, conducting tutorials, examination invigilation, setting questions, and paper marking for undergraduates

2013 Sep—2014 Jan: Trainee laboratory analyst (intern). national water supply & drainage board.
Responsibilities: water quality testing for chemical parameters and bacteriological parameters, site inspections, laboratory chemical stock maintenances.

MEMBERSHIPS

- Texas Academy of Science (TAS)
- Sri Lankan American Knowledge Exchange (SLAKE)